

Supporting Information

Selective C-F and C-H Activation of Fluoroarenes by Fe(PMe₃)₄ and Catalytic Performance of Iron Hydride in Hydrosilylation of Carbonyl Compounds

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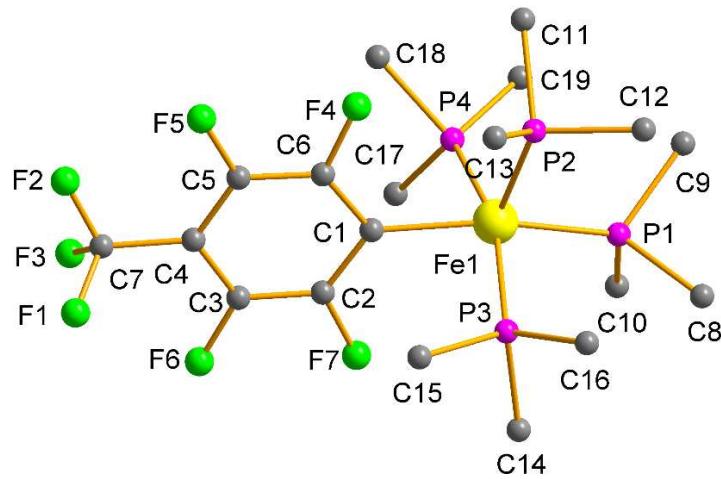
(1) Stick-ball representations and Cartesian coordinates of complexes **1** and **3**

(2) IR spectra of complexes **1 - 4** and **6**

(3) ¹H NMR, ³¹P NMR, ¹⁹F NMR and ¹³C NMR spectra of complexes **4** and **6**

(4) ¹H NMR and ¹³C NMR spectra of the catalytic products (alcohols)

(1) Stick-ball representations and Cartesian coordinates of complexes **1** and **3**



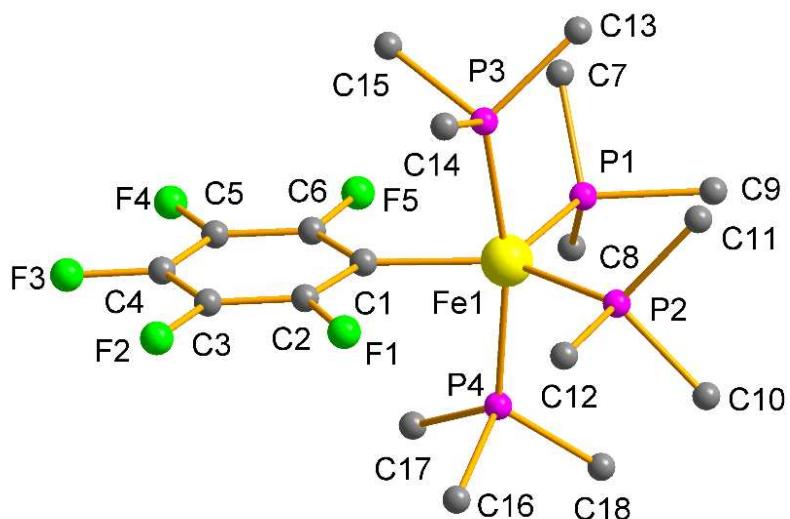
Complex **1**

Atomic coordinates ($x \times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for complex **1**.

$U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Fe(1)	2137(1)	6812(1)	1236(1)	16(1)
P(1)	1141(1)	7922(1)	1684(1)	20(1)
P(2)	3383(1)	7398(1)	2207(1)	22(1)
P(3)	2301(1)	8500(1)	468(1)	24(1)
P(4)	1752(1)	4778(1)	1620(1)	21(1)
C(1)	2685(2)	5544(3)	592(2)	19(1)
C(2)	2219(2)	5162(3)	-158(2)	20(1)
C(3)	2535(3)	4242(3)	-596(2)	21(1)
C(4)	3372(3)	3602(3)	-322(2)	25(1)
C(5)	3878(3)	3968(3)	409(2)	27(1)
C(6)	3526(3)	4878(3)	832(2)	23(1)
C(7)	3683(4)	2577(4)	-808(2)	38(1)
C(8)	979(3)	9806(3)	1620(2)	32(1)
C(9)	1157(3)	7774(4)	2698(2)	31(1)
C(10)	-43(3)	7461(3)	1204(2)	32(1)
C(11)	3817(3)	6232(3)	3025(2)	32(1)
C(12)	3287(3)	8950(3)	2754(2)	33(1)

C(13)	4465(3)	7877(4)	2030(2)	37(1)
C(14)	1276(4)	8979(4)	-290(2)	40(1)
C(15)	3083(4)	8222(4)	-109(3)	41(1)
C(16)	2715(3)	10240(3)	808(2)	37(1)
C(17)	912(3)	3835(3)	866(2)	33(1)
C(18)	2607(3)	3401(3)	1934(2)	30(1)
C(19)	1217(4)	4541(4)	2390(3)	40(1)
F(1)	3765(3)	3094(3)	-1439(2)	59(1)
F(2)	4381(3)	1853(3)	-446(2)	77(1)
F(3)	3018(3)	1583(2)	-1065(2)	60(1)
F(4)	4081(2)	5051(2)	1555(1)	32(1)
F(5)	4703(2)	3423(3)	730(1)	45(1)
F(6)	2009(2)	3972(2)	-1312(1)	29(1)
F(7)	1392(2)	5703(2)	-524(1)	28(1)



Complex 3

Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for complex 3.

$U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Fe(1)	8091(1)	2374(1)	6314(1)	15(1)
P(1)	7164(1)	2012(1)	7528(1)	27(1)

P(2)	7152(1)	1557(1)	5328(1)	27(1)
P(3)	6441(1)	3313(1)	6027(1)	25(1)
P(4)	10060(1)	1631(1)	6503(1)	25(1)
F(1)	9821(1)	3305(1)	4940(1)	33(1)
F(2)	11658(2)	4522(1)	5028(1)	44(1)
F(3)	12406(2)	5232(1)	6534(1)	49(1)
F(4)	11219(2)	4698(1)	7946(1)	40(1)
F(5)	9355(2)	3495(1)	7882(1)	41(1)
C(1)	9472(2)	3318(1)	6407(1)	20(1)
C(2)	10124(2)	3629(1)	5715(1)	22(1)
C(3)	11080(2)	4258(1)	5737(1)	27(1)
C(4)	11458(2)	4621(1)	6486(1)	29(1)
C(5)	10858(2)	4345(1)	7201(1)	26(1)
C(6)	9897(2)	3720(1)	7139(1)	25(1)
C(7)	6143(4)	2728(2)	8136(2)	66(1)
C(8)	8325(3)	1681(2)	8423(1)	44(1)
C(9)	5898(3)	1167(2)	7509(2)	56(1)
C(10)	7463(3)	465(1)	5297(2)	53(1)
C(11)	5229(2)	1499(2)	5050(2)	43(1)
C(12)	7786(3)	1798(2)	4277(1)	47(1)
C(13)	4514(2)	3143(2)	6153(2)	47(1)
C(14)	6366(3)	3719(1)	4960(2)	41(1)
C(15)	6646(3)	4276(1)	6585(2)	46(1)
C(16)	11175(2)	1552(2)	5597(2)	43(1)
C(17)	11448(2)	1981(2)	7274(2)	40(1)
C(18)	10015(3)	562(1)	6814(2)	46(1)

(2) IR spectra of complexes **1 – 4** and **6**

Figure S1 IR spectrum of complex **1**

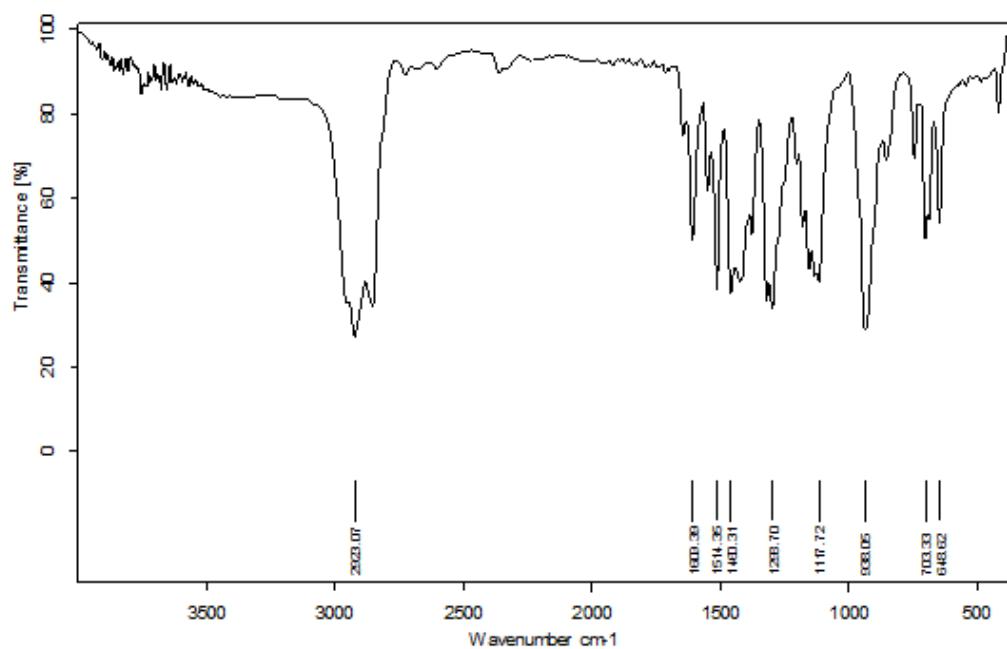


Figure S2 IR spectrum of complex **2**

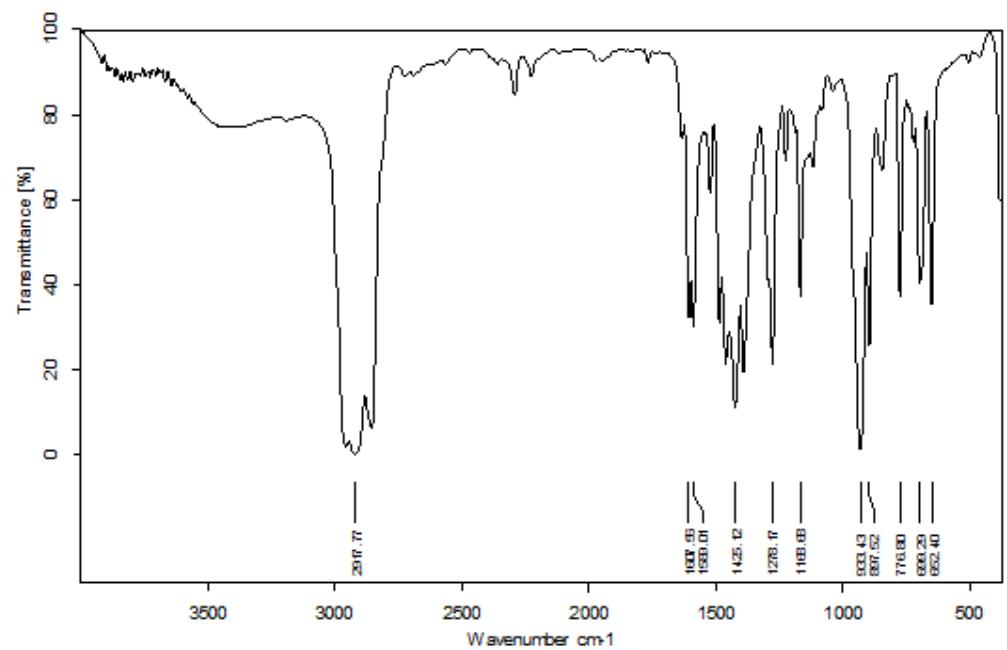


Figure S3 IR spectrum of complex 3

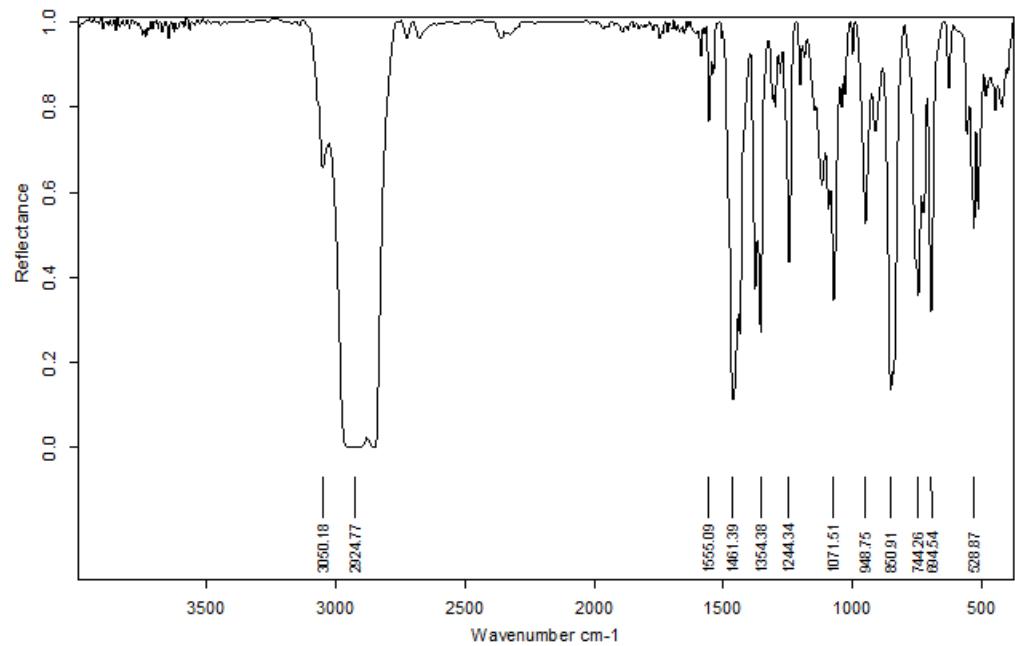


Figure S4 IR spectrum of complex 4

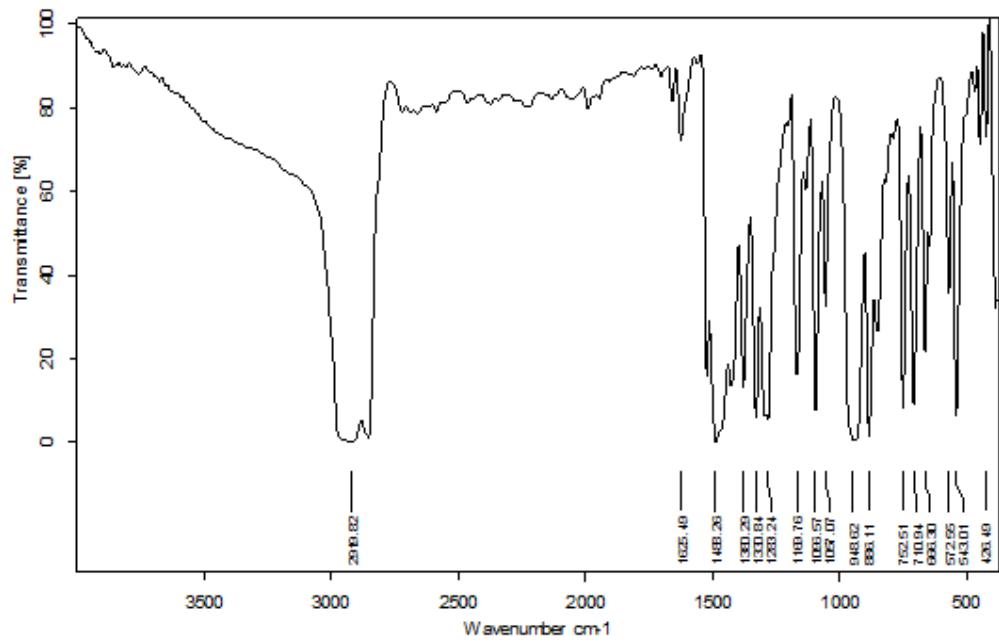
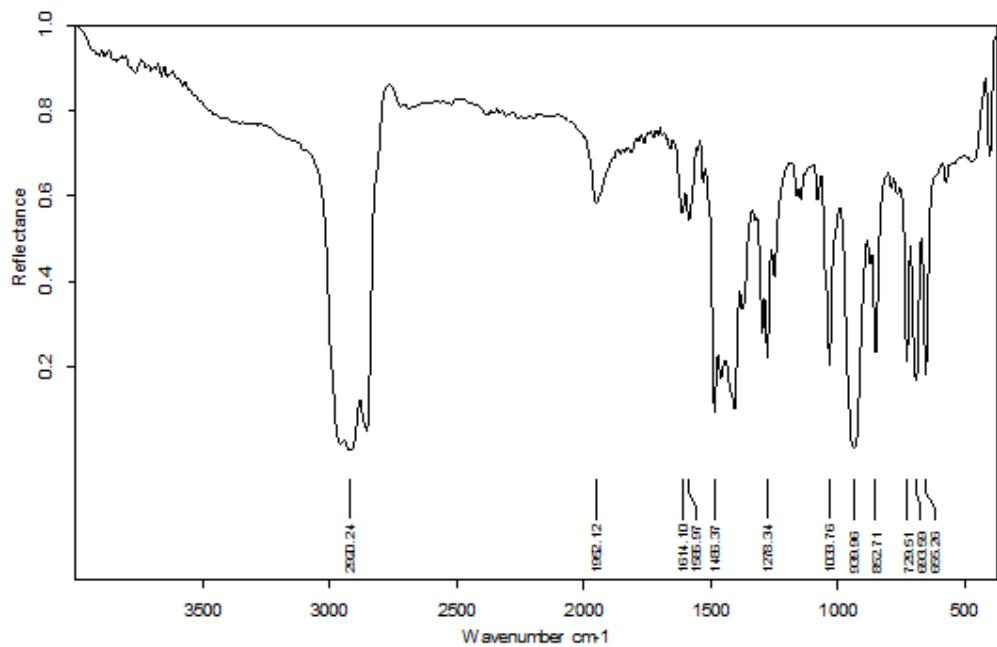


Figure S5 IR spectrum of complex 6



(3) ^1H NMR, ^{31}P NMR, ^{19}F NMR and ^{13}C NMR spectra of complexes 4 and 6

Figure S6 ^1H NMR of complex 4

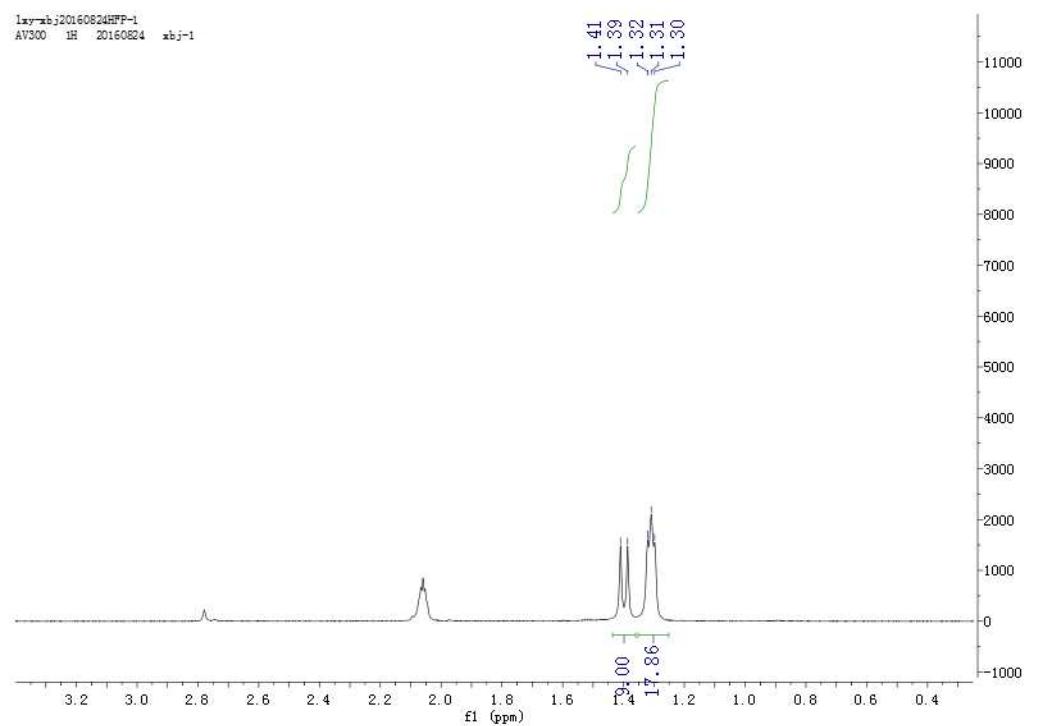


Figure S7 ^{31}P NMR of complex 4

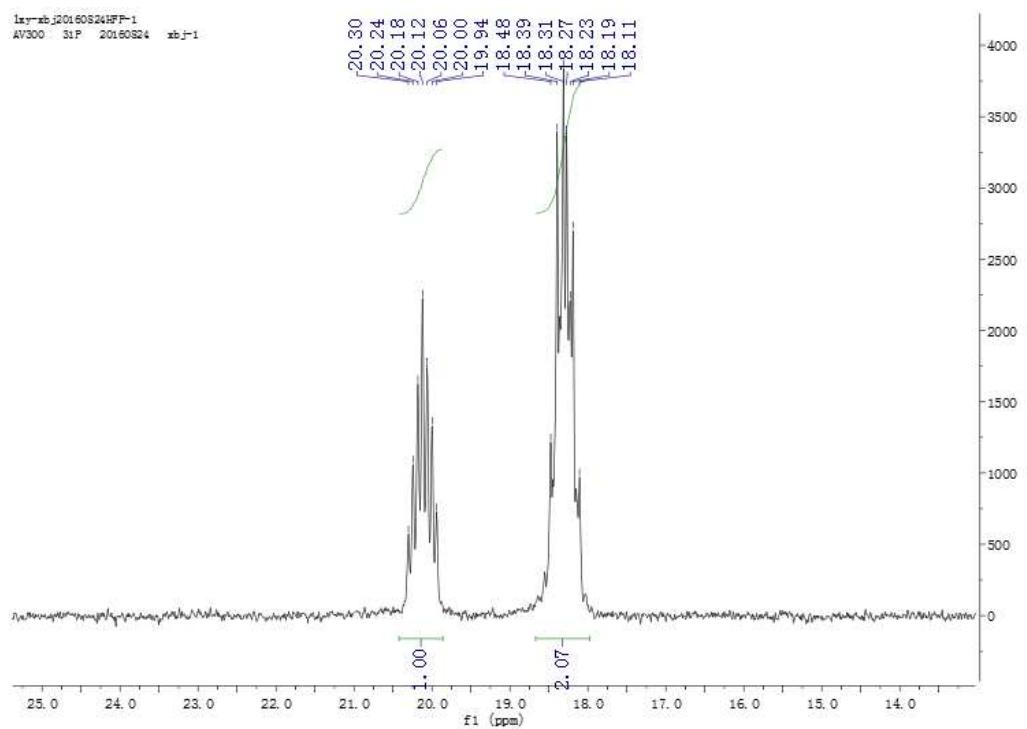


Figure S8 ^{19}F NMR of complex 4

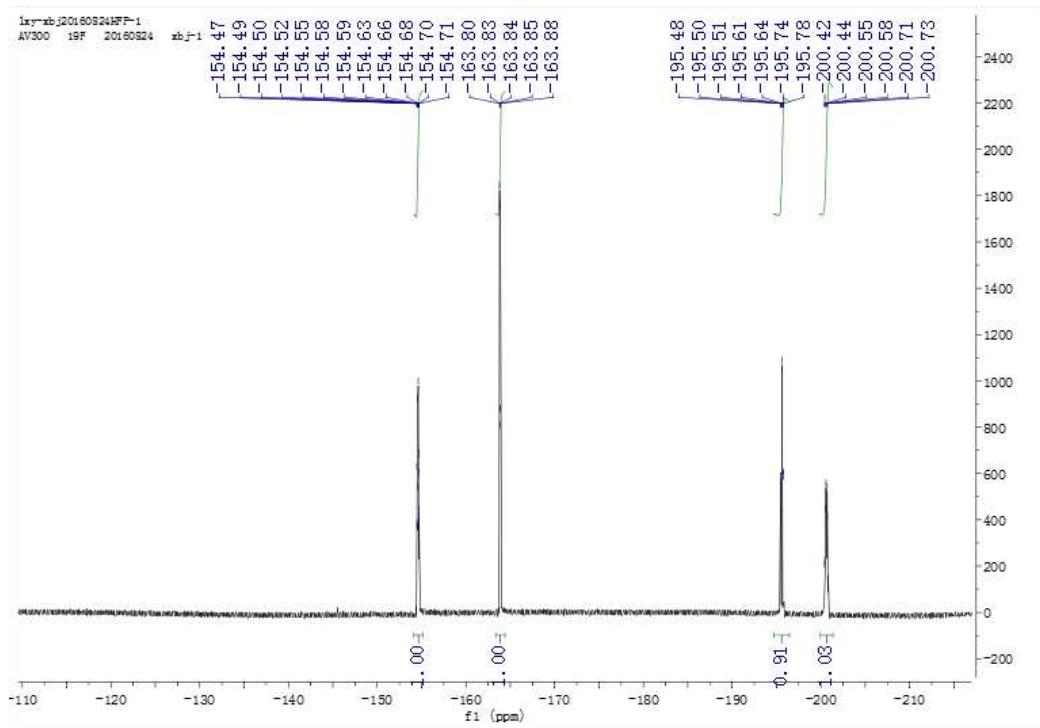


Figure S9 ^{13}C NMR of complex 4

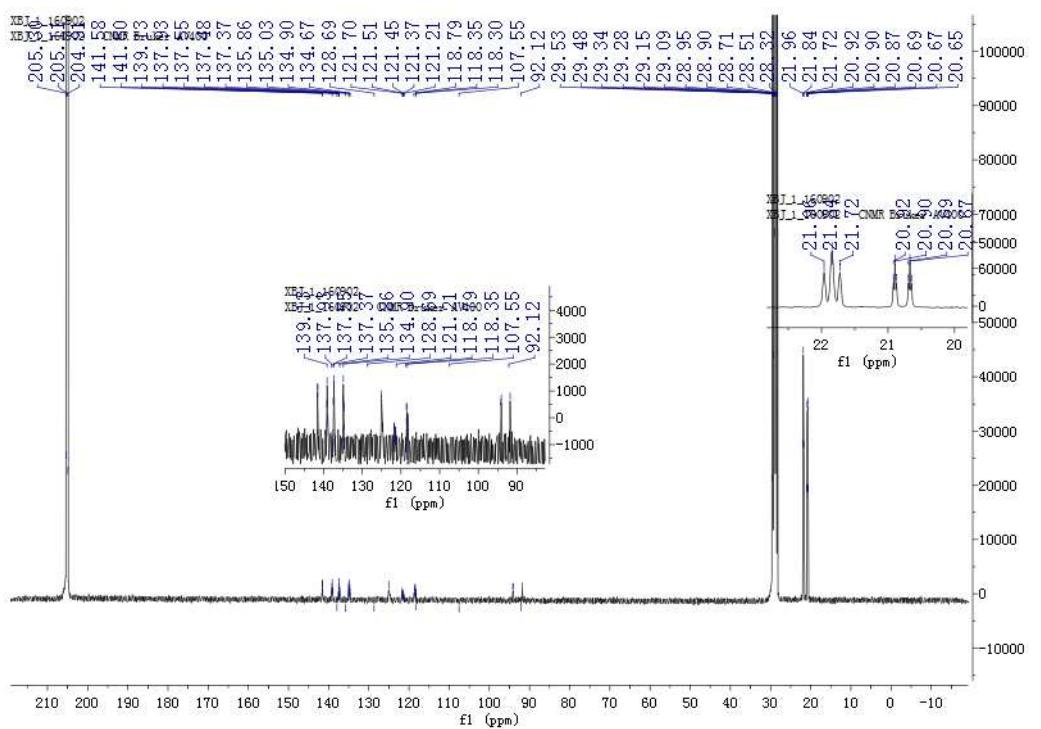


Figure S10 ^1H NMR of complex 4 at -45°C

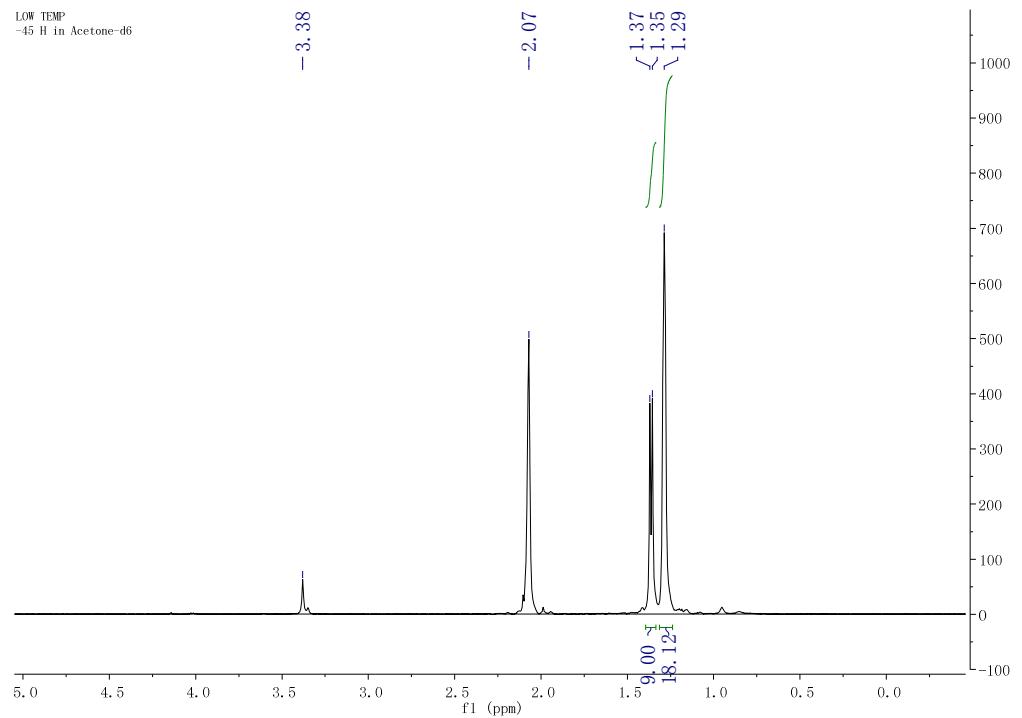


Figure S11 ^{31}P NMR of complex 4 at -45°C

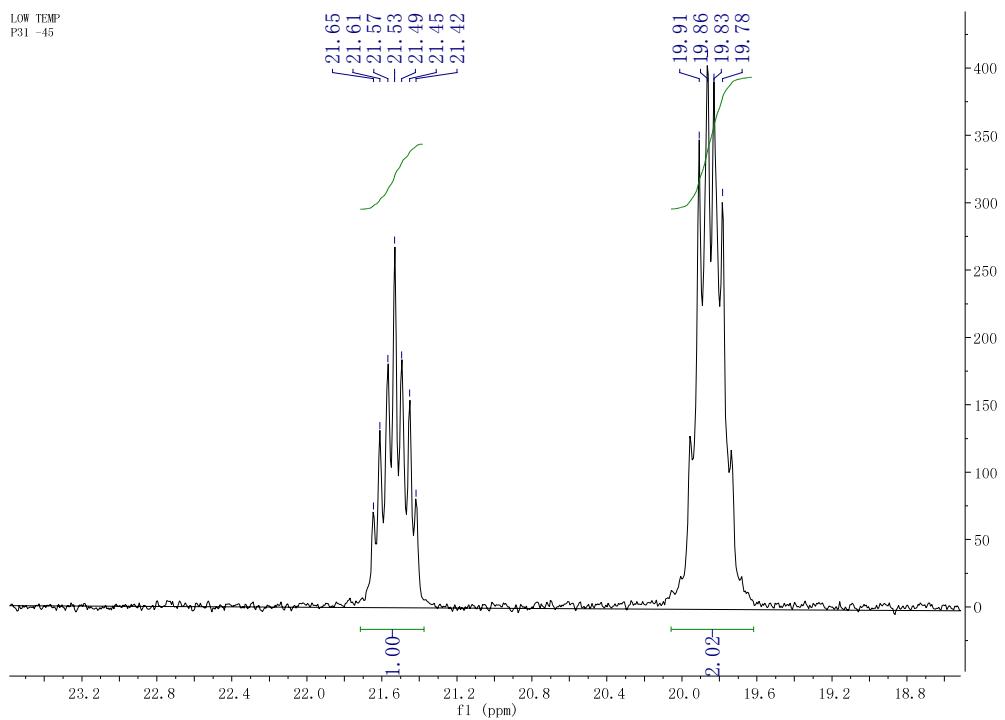


Figure S12 ^{19}F NMR of complex 4 at -45°C

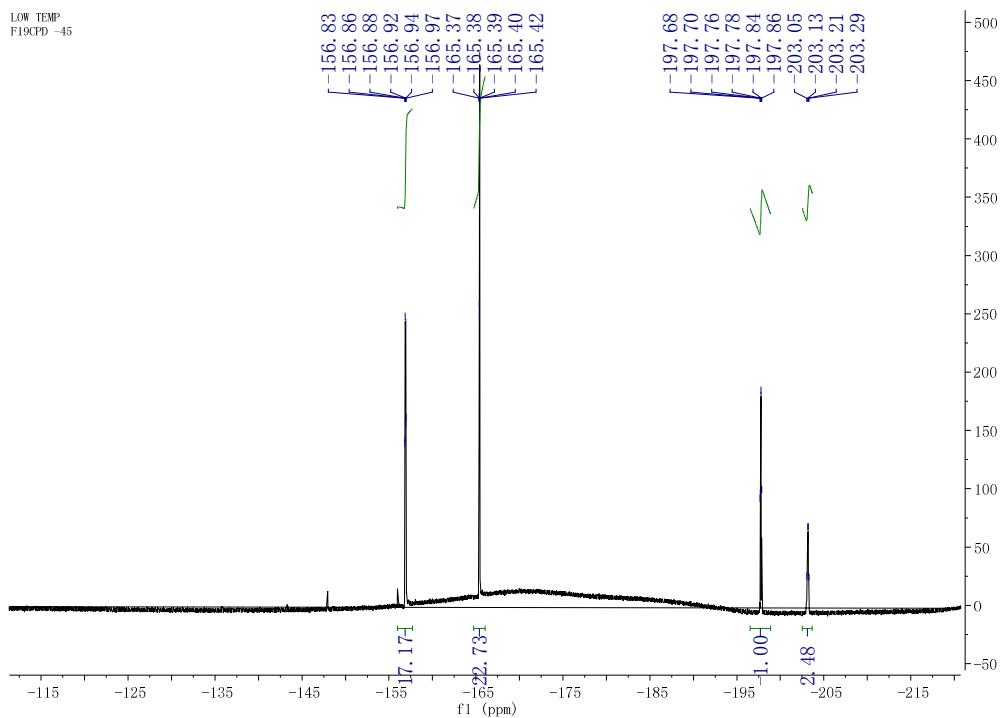


Figure S13 ^1H NMR of complex 6

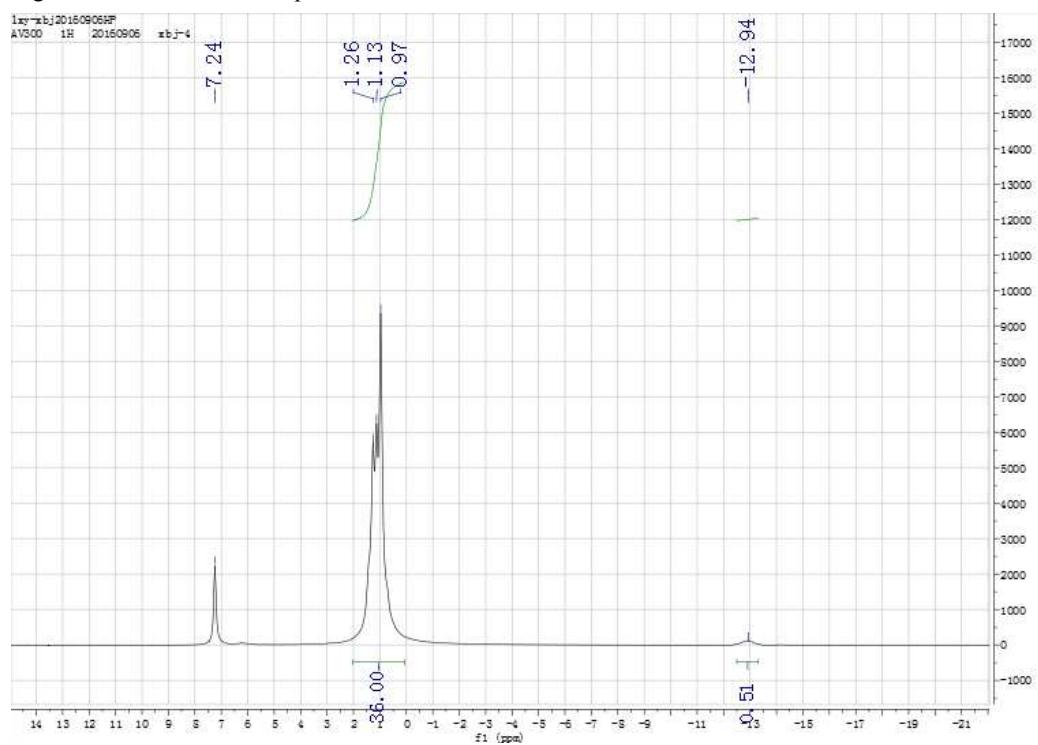


Figure S14 ^{31}P NMR of complex 6

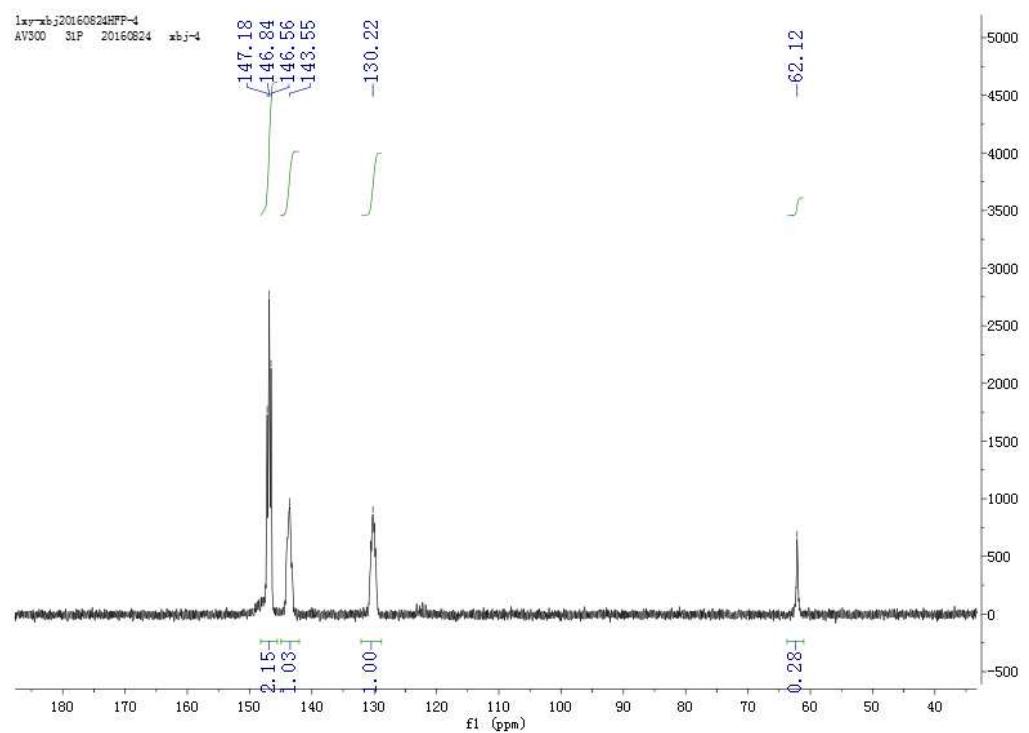


Figure S15 ^{19}F NMR of complex 6

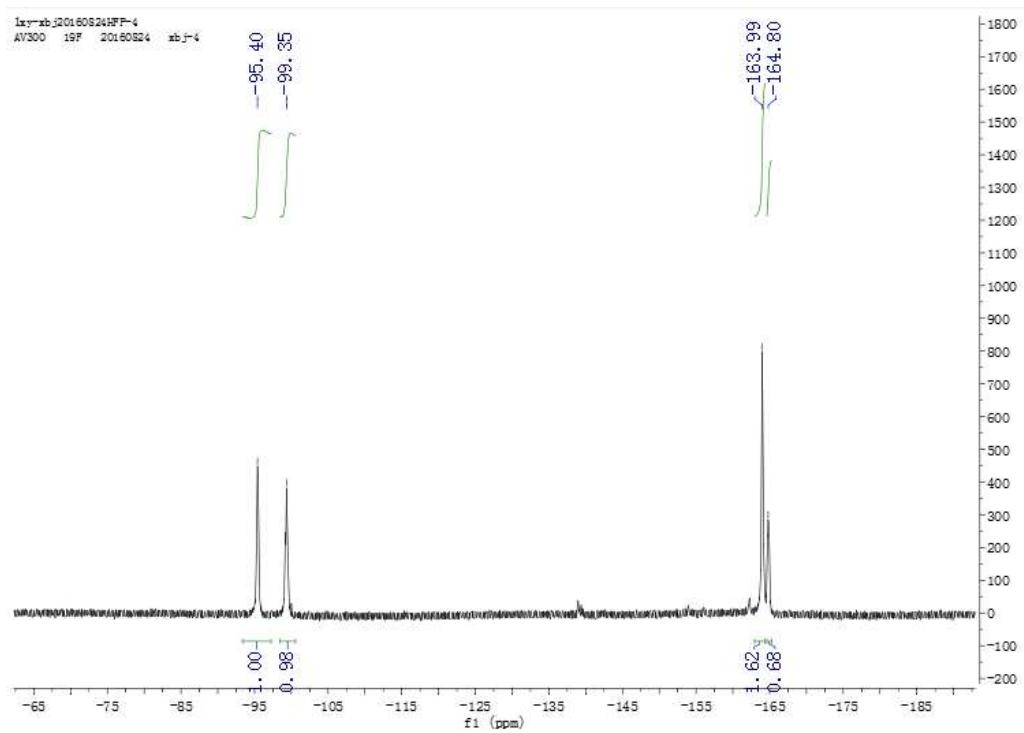
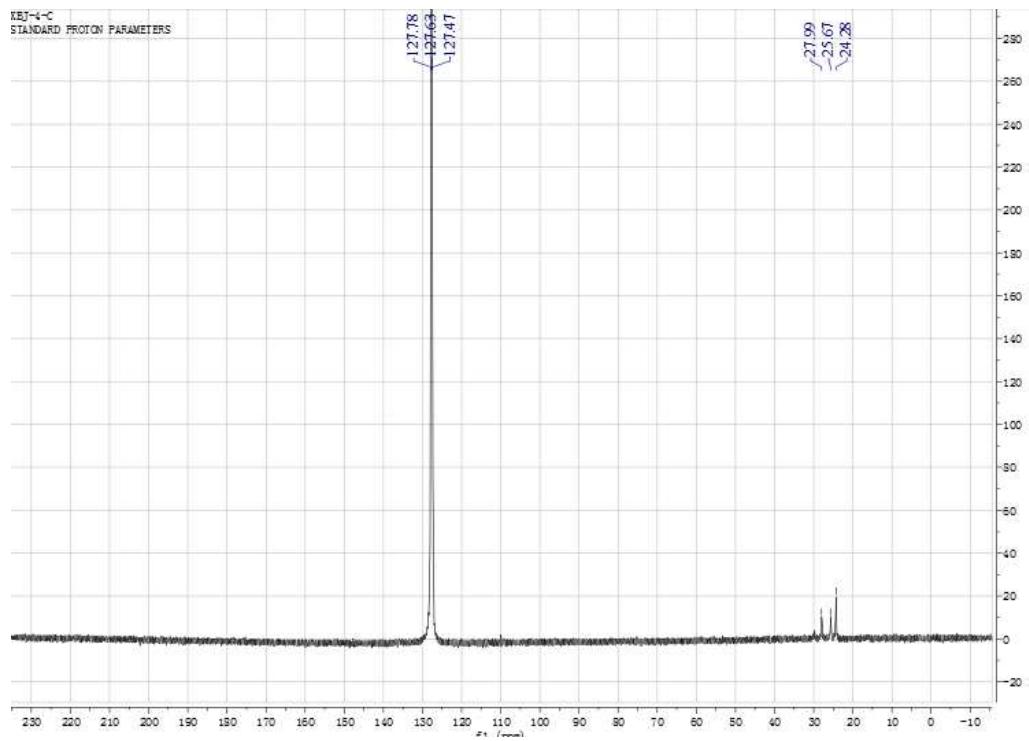
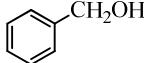


Figure S16 ^{13}C NMR of complex 6



(4) ^1H NMR and ^{13}C NMR spectra of the catalytic products (alcohols)

Figure S17 ^1H NMR of compound 

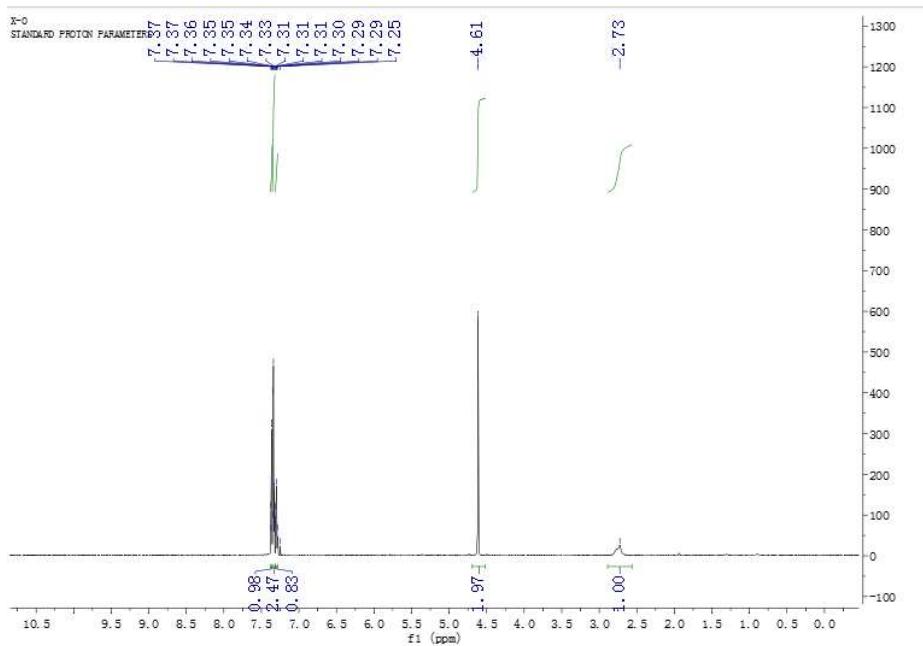
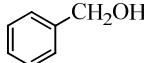


Figure S18 ^{13}C NMR of compound 

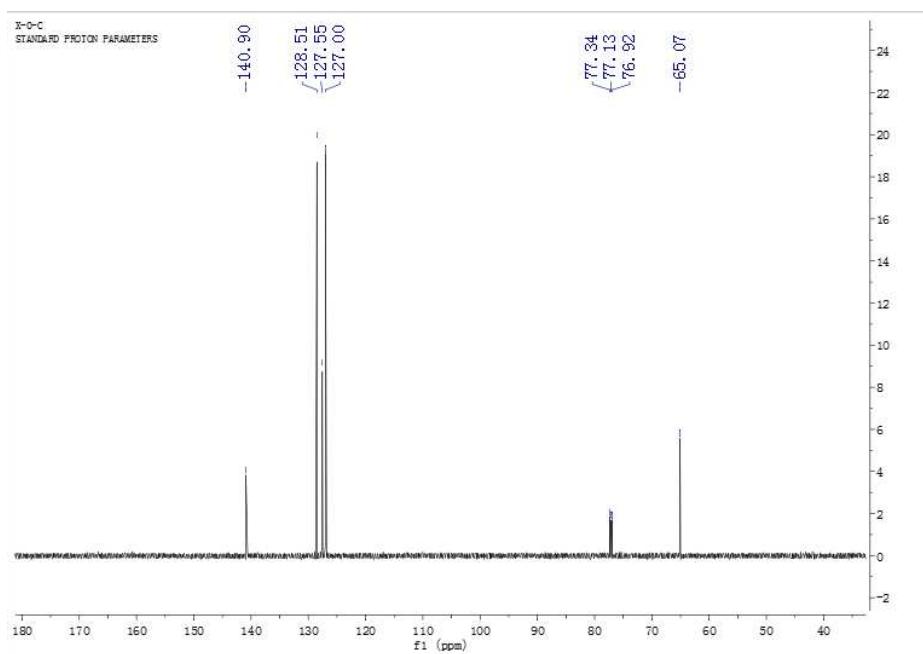
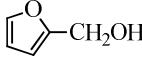


Figure S19 ^1H NMR of compound 

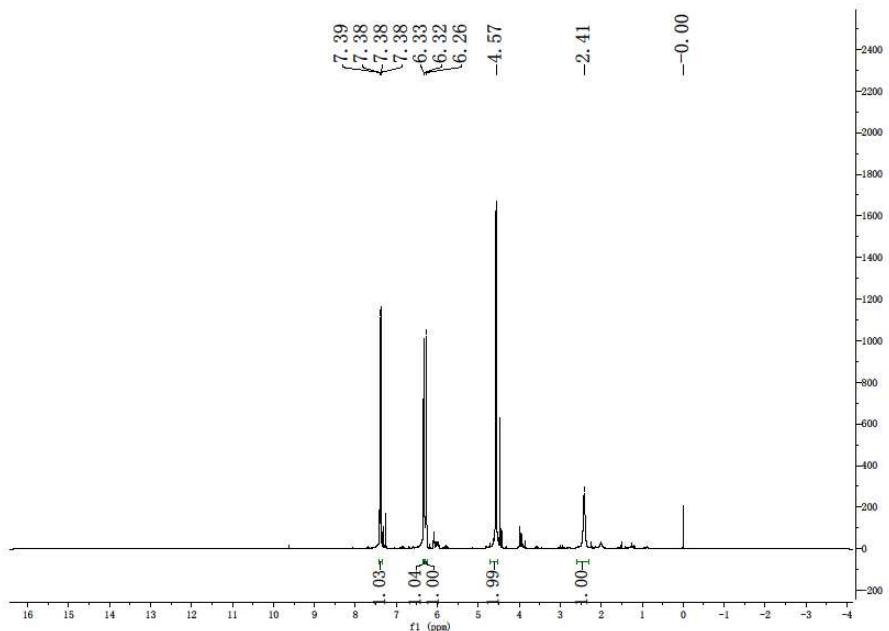


Figure S20 ^{13}C NMR of compound 

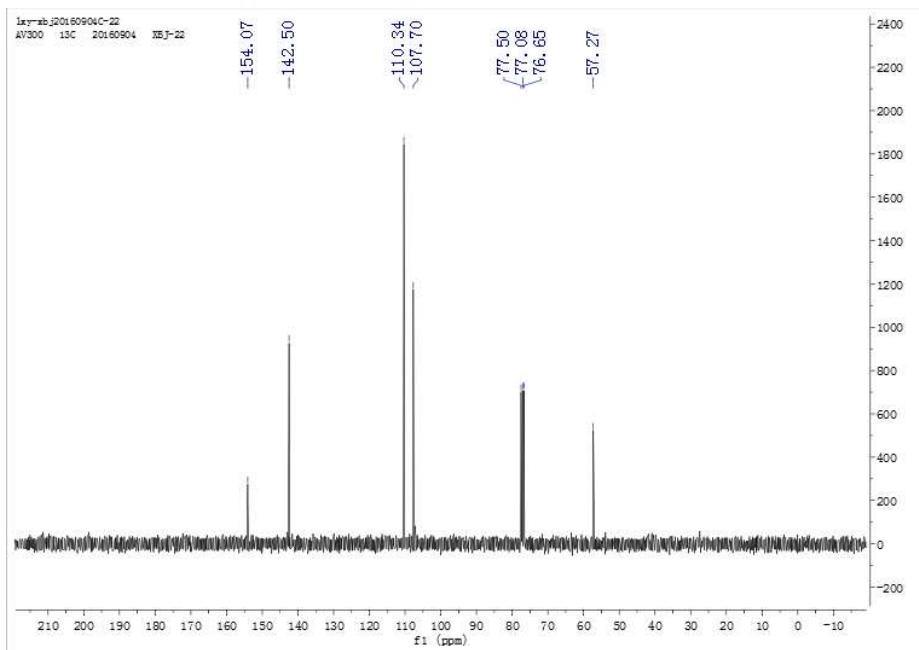
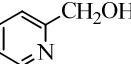


Figure S21 ^1H NMR of compound 

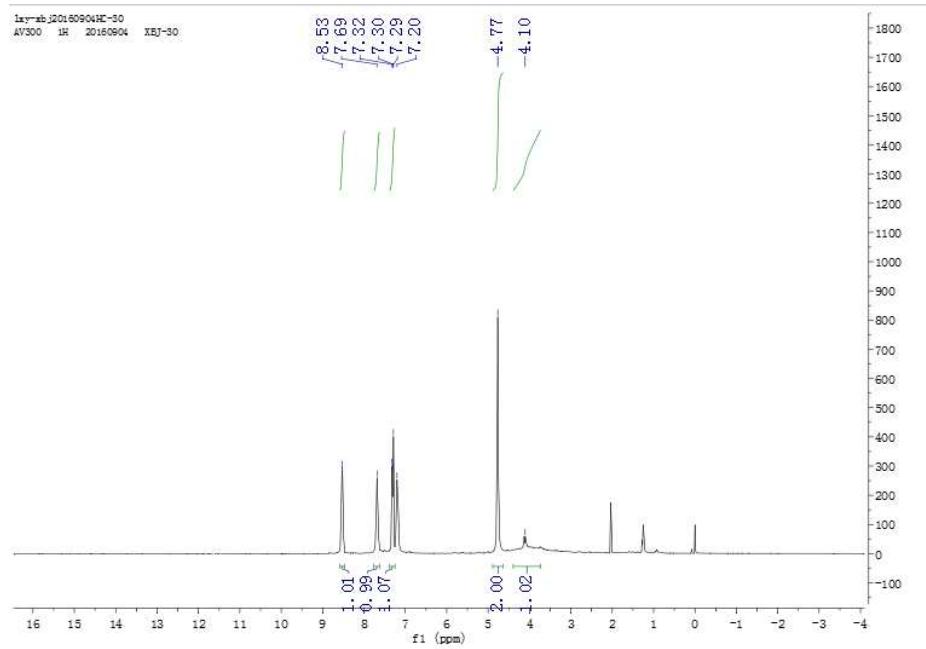


Figure S22 ^{13}C NMR of compound 

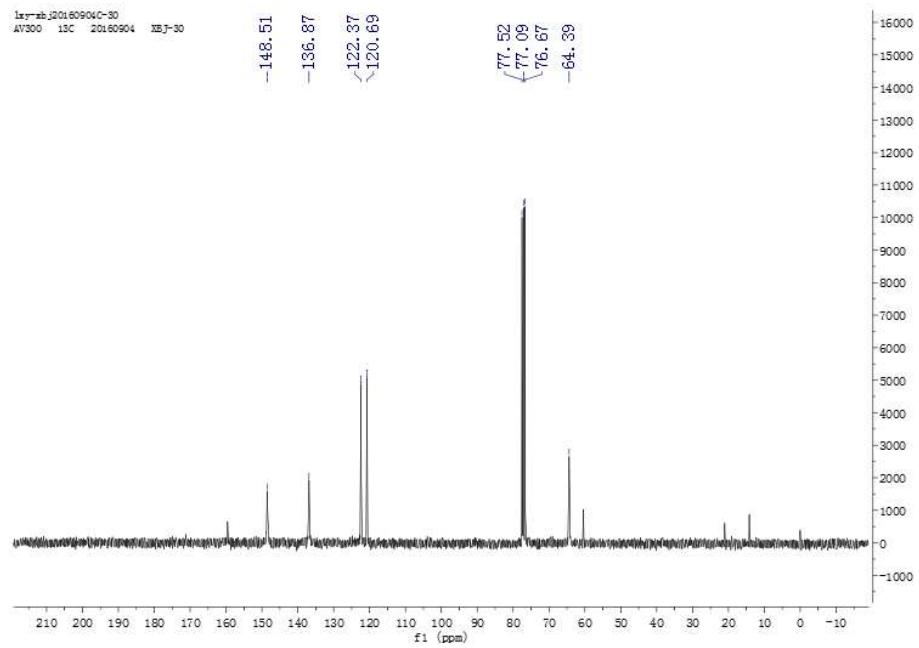
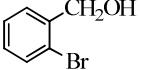


Figure S23 ^1H NMR of compound 

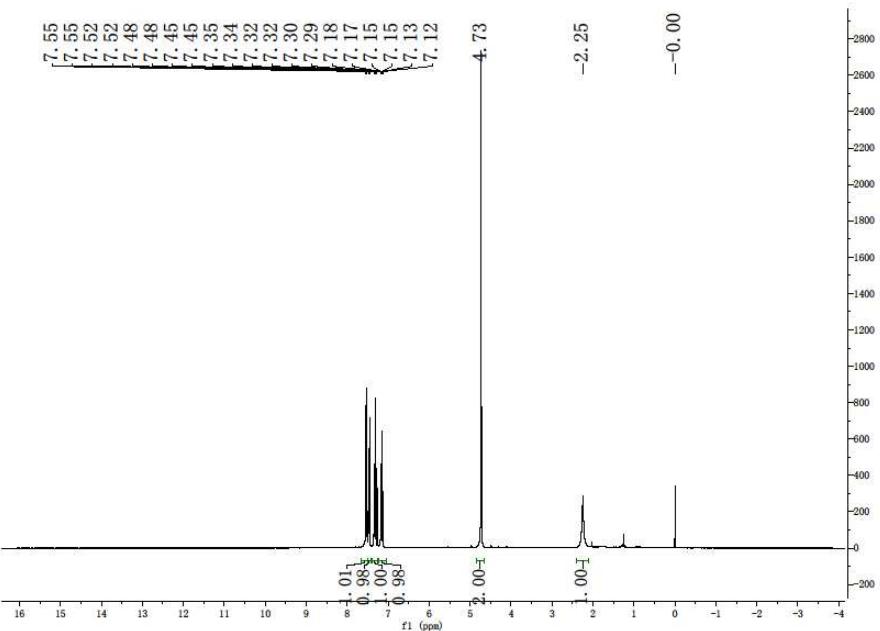
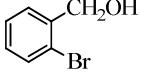


Figure S24 ^{13}C NMR of compound 

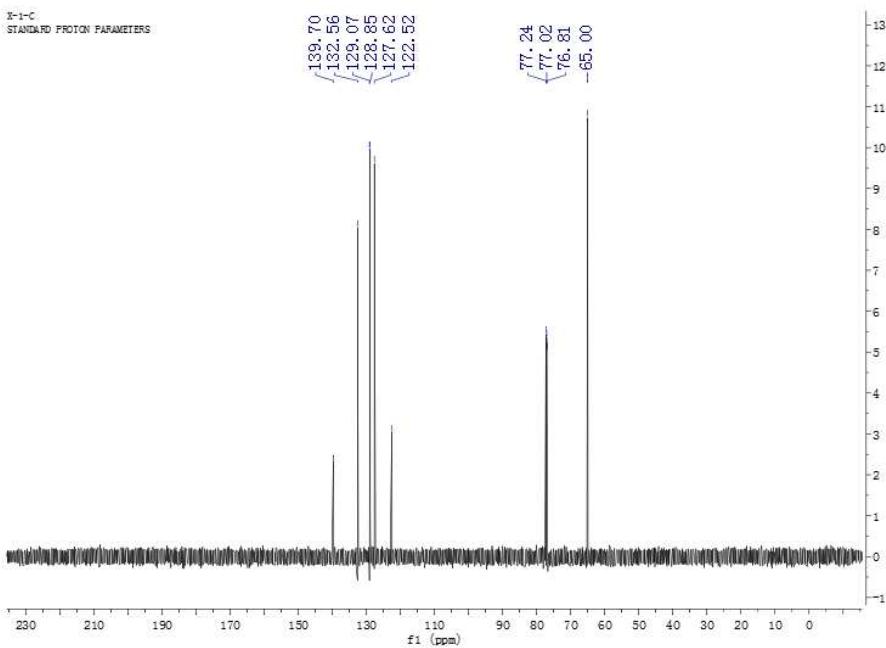
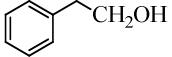


Figure S25 ^1H NMR of compound 

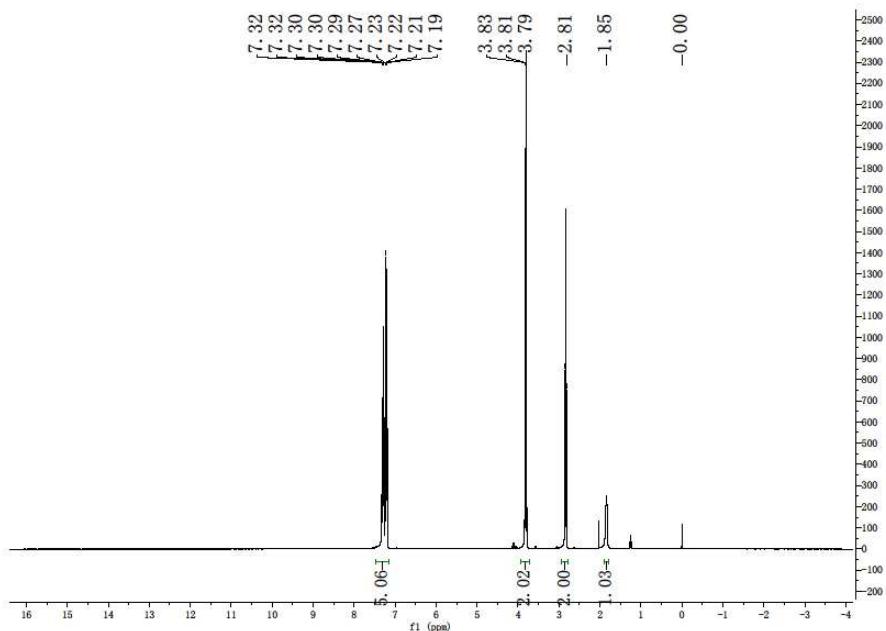
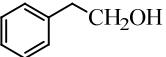


Figure S26 ^{13}C NMR of compound 

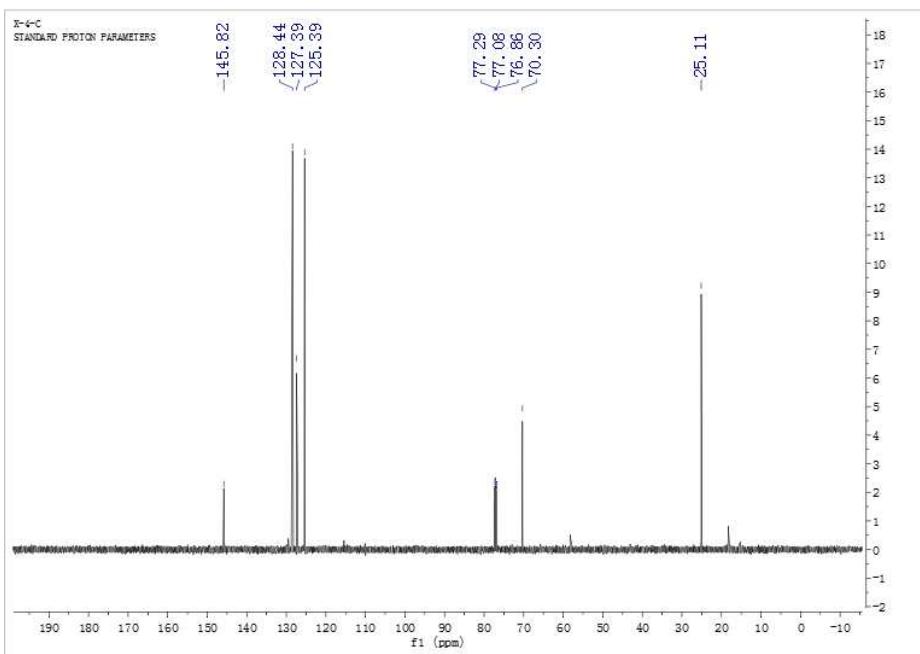


Figure S27 ^1H NMR of compound

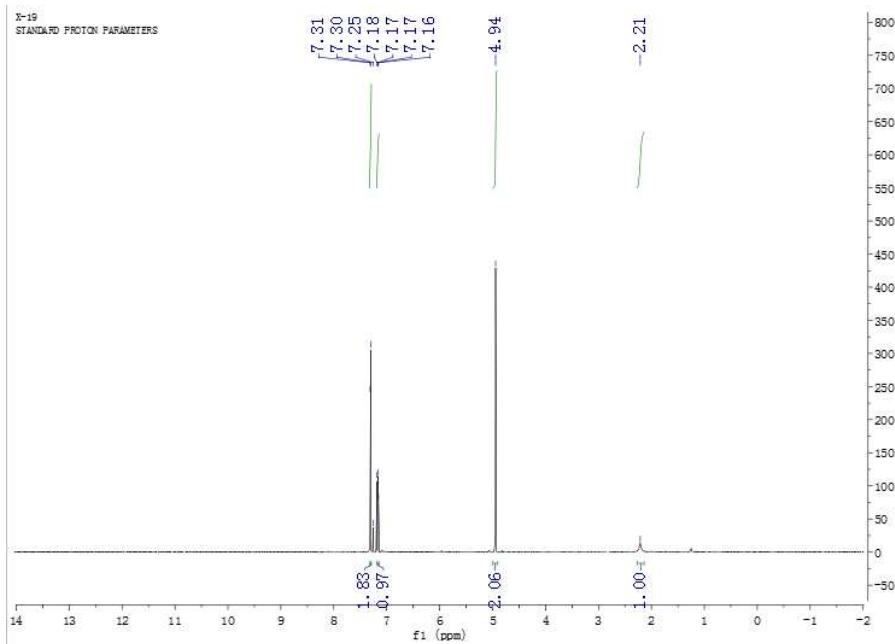
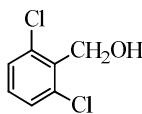


Figure S28 ^{13}C NMR of compound

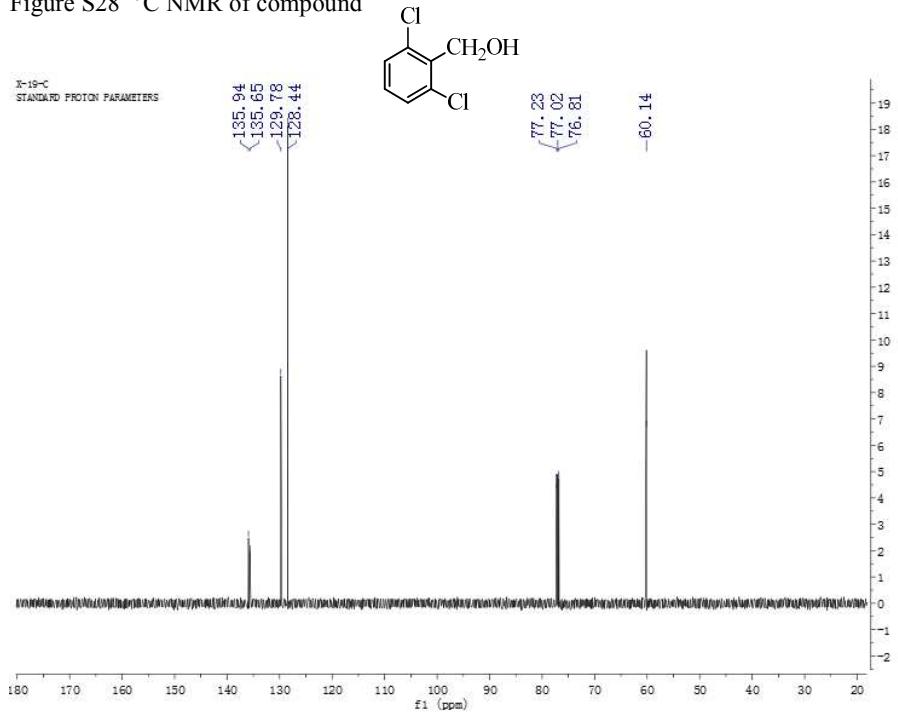
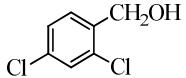


Figure S29 ^1H NMR of compound 

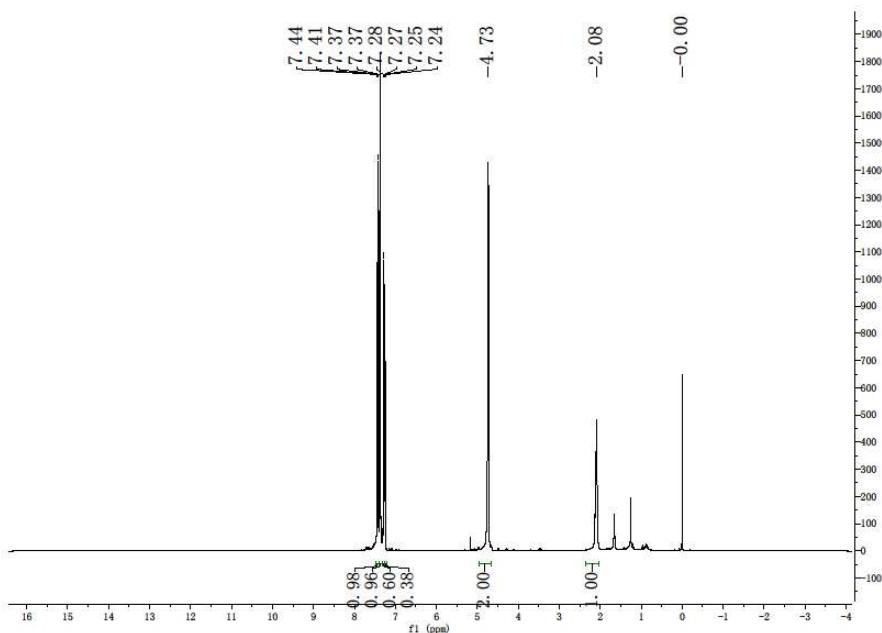
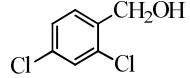


Figure S30 ^{13}C NMR of compound 

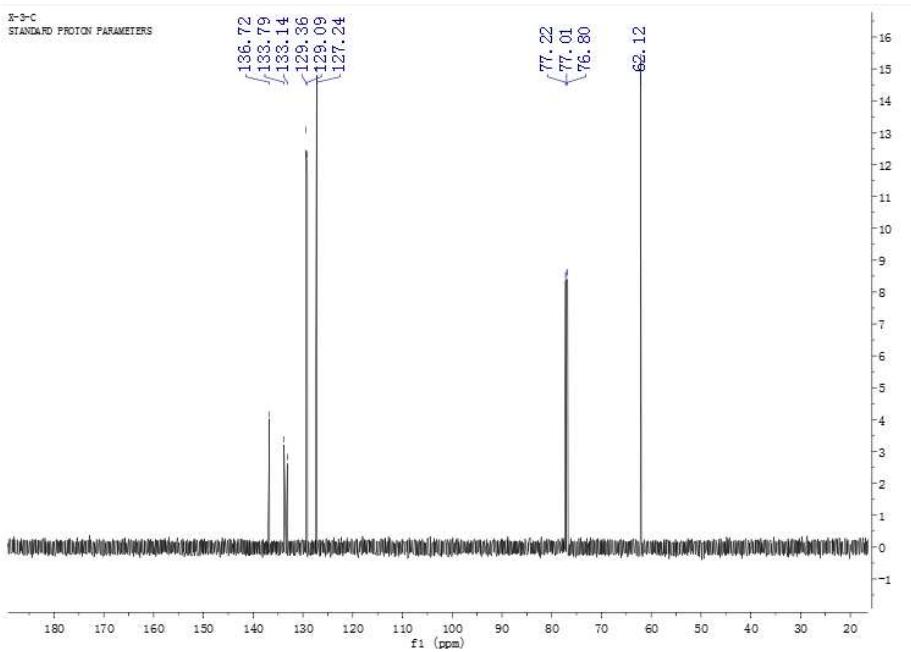
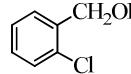


Figure S31 ^1H NMR of compound 

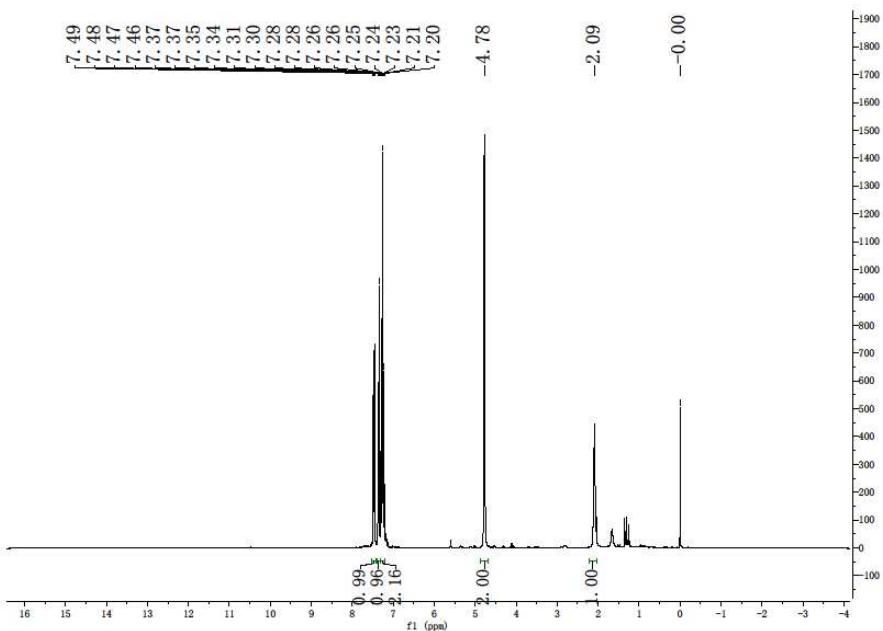
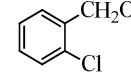
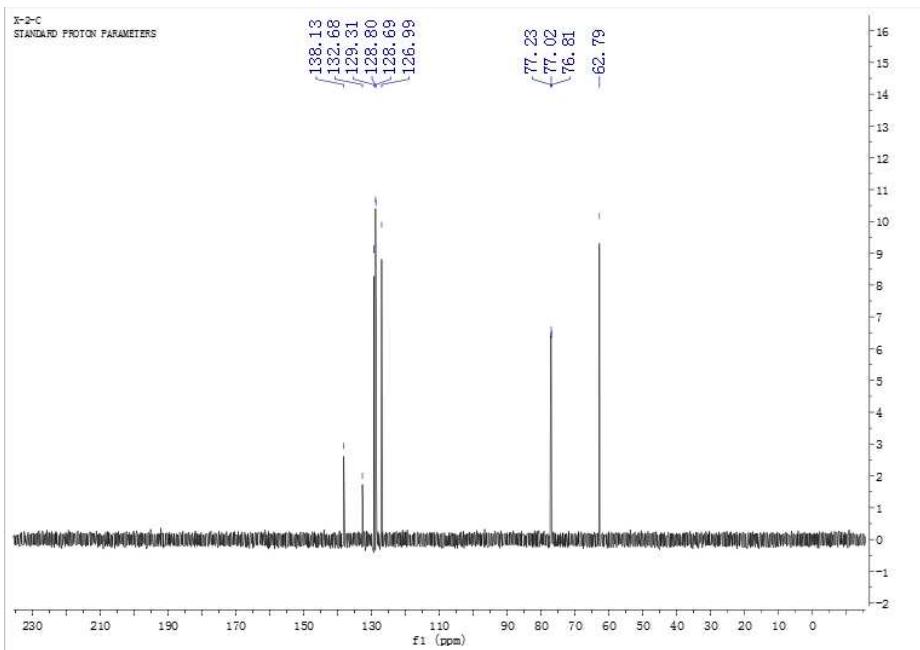


Figure S32 ^{13}C NMR of compound 



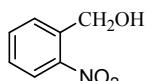


Figure S33 ^1H NMR of compound

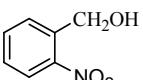
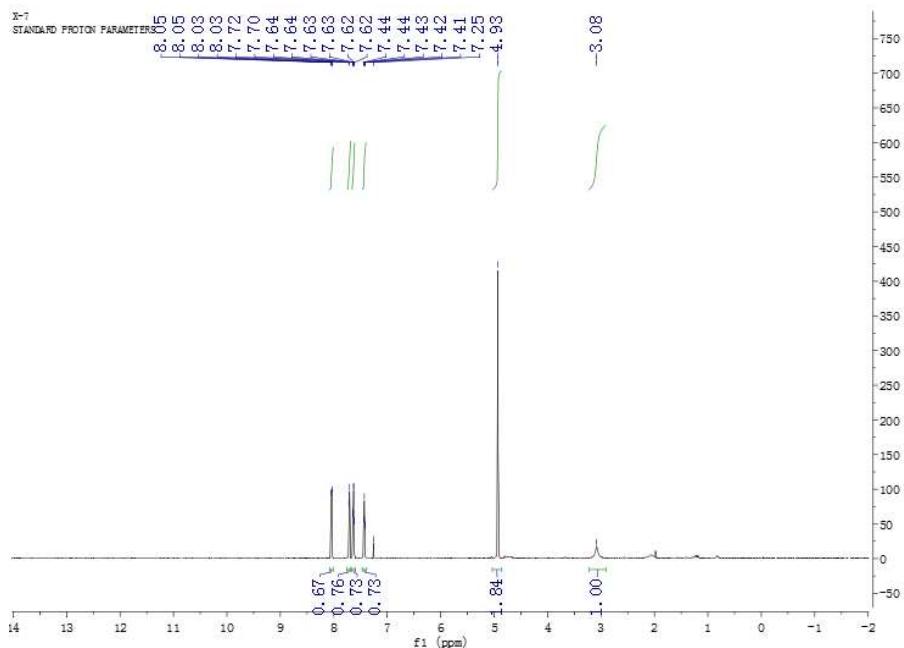
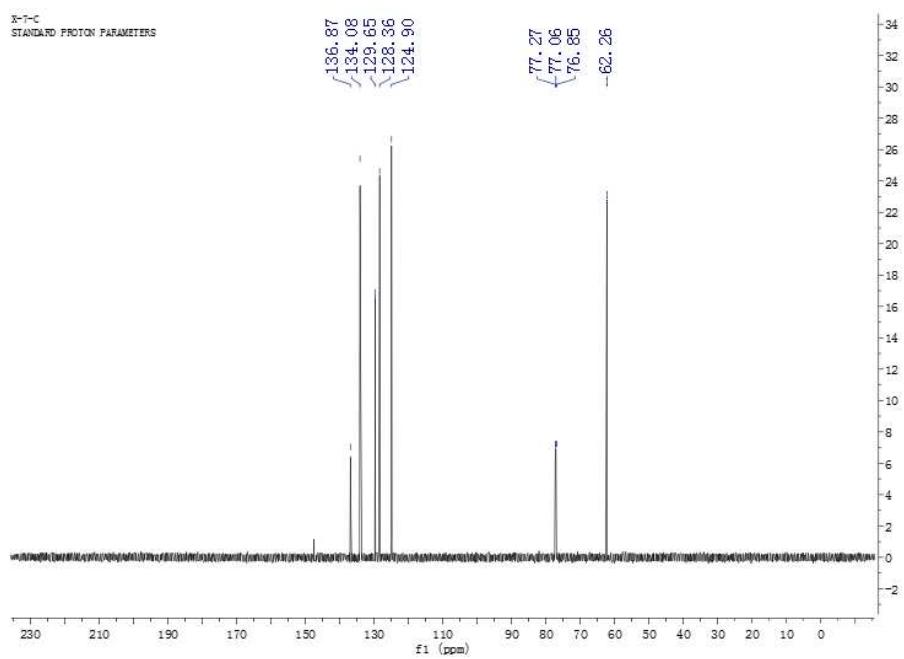
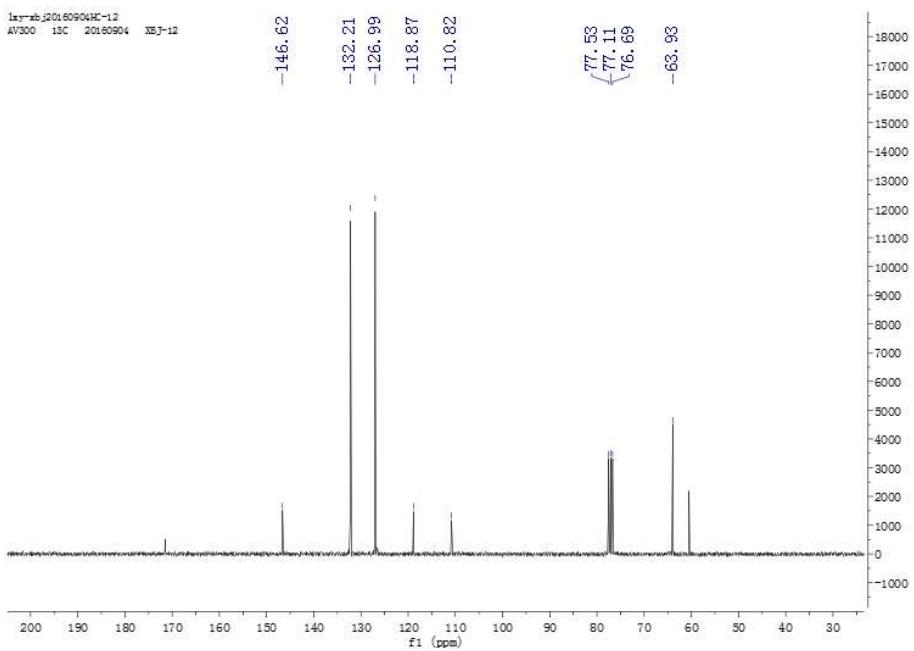
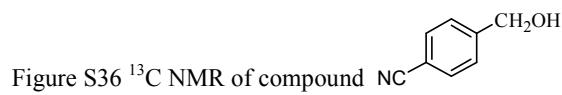
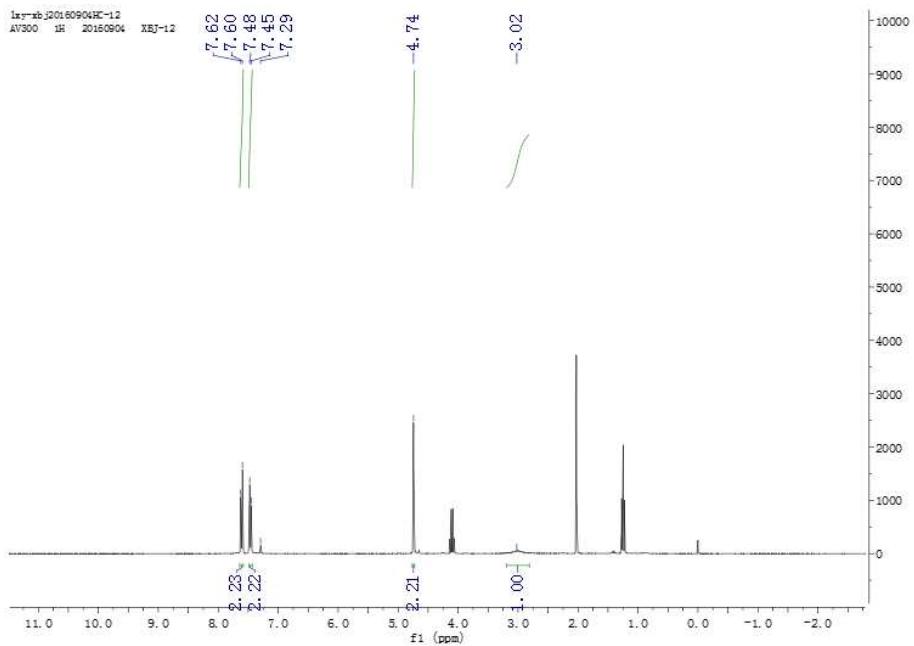
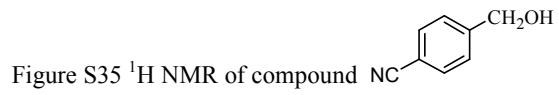


Figure S34 ^{13}C NMR of compound





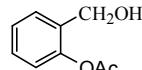


Figure S37 ^1H NMR of compound

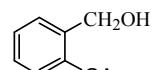
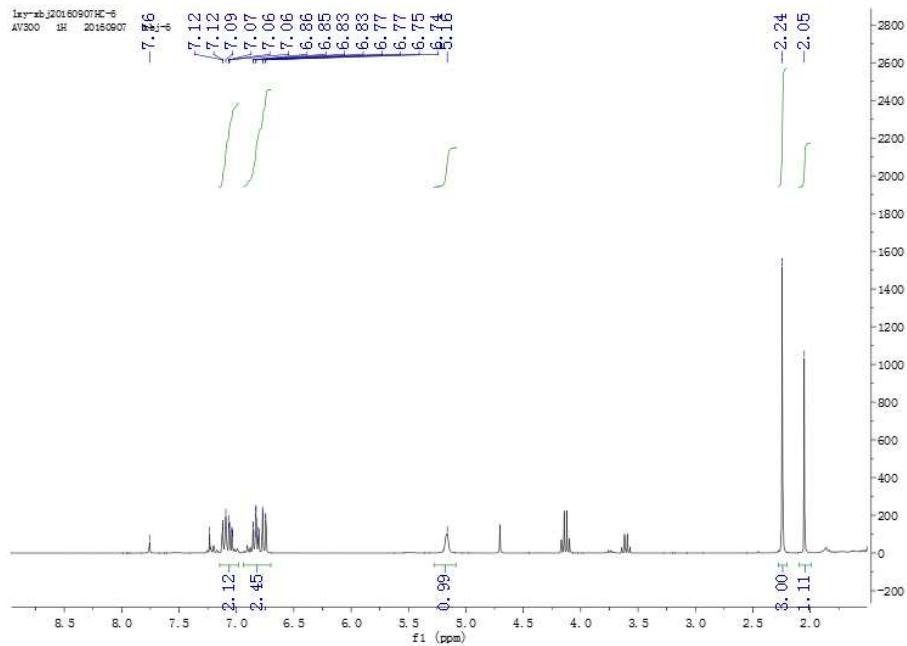


Figure S38 ^{13}C NMR of compound

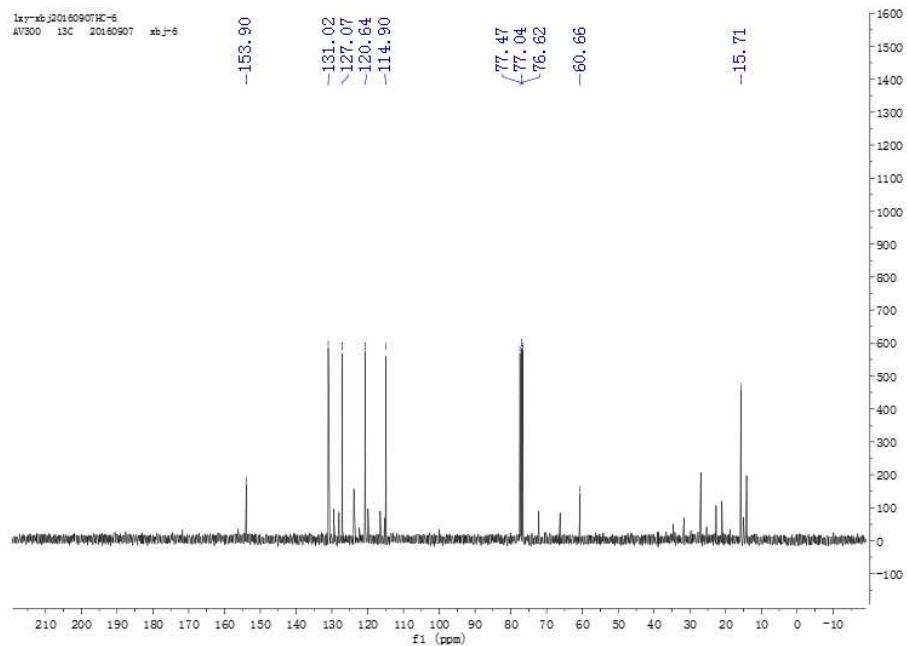


Figure S39 ^1H NMR of compound

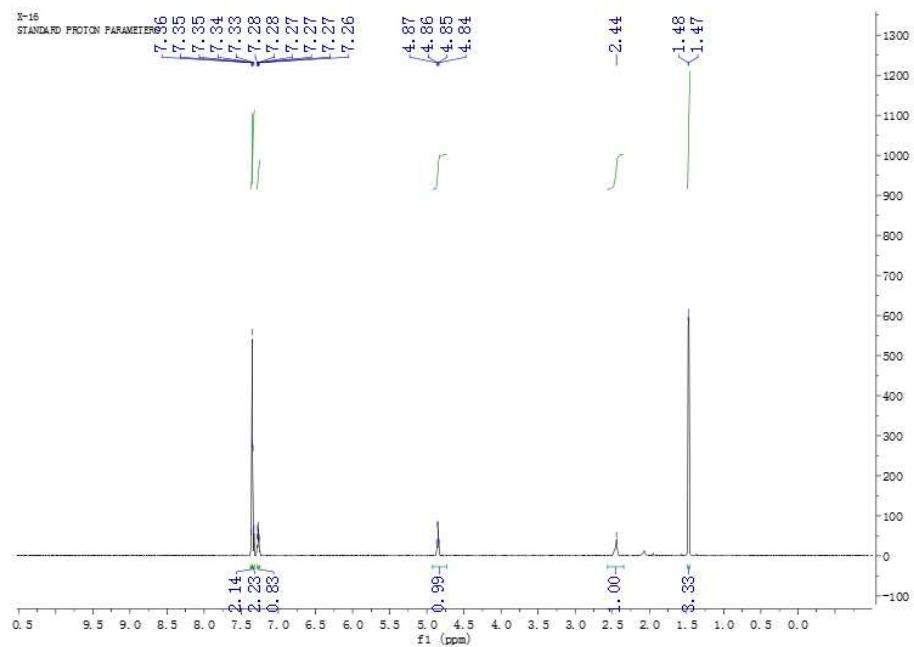


Figure S40 ^{13}C NMR of compound

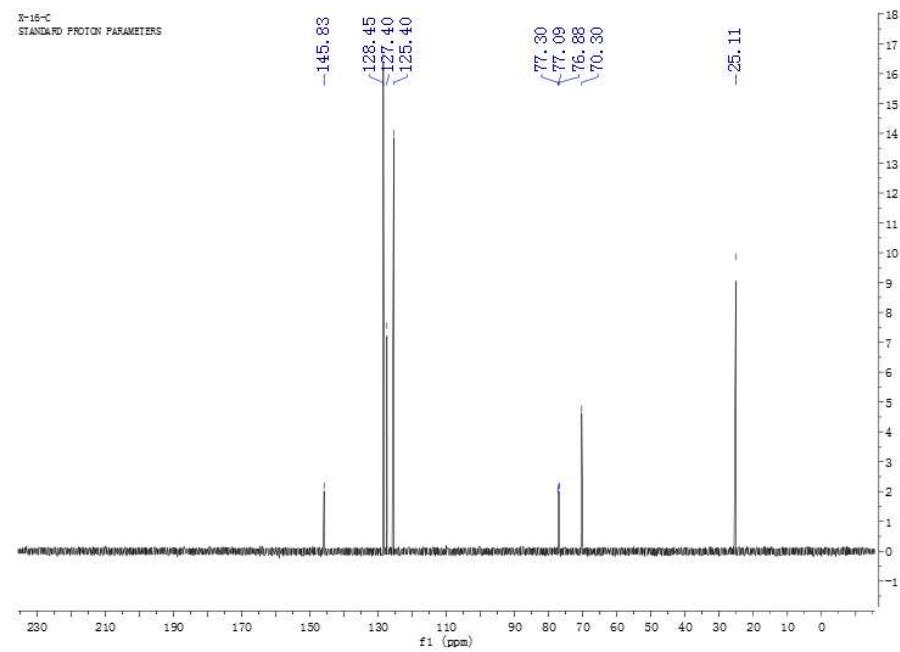


Figure S41 ^1H NMR of compound

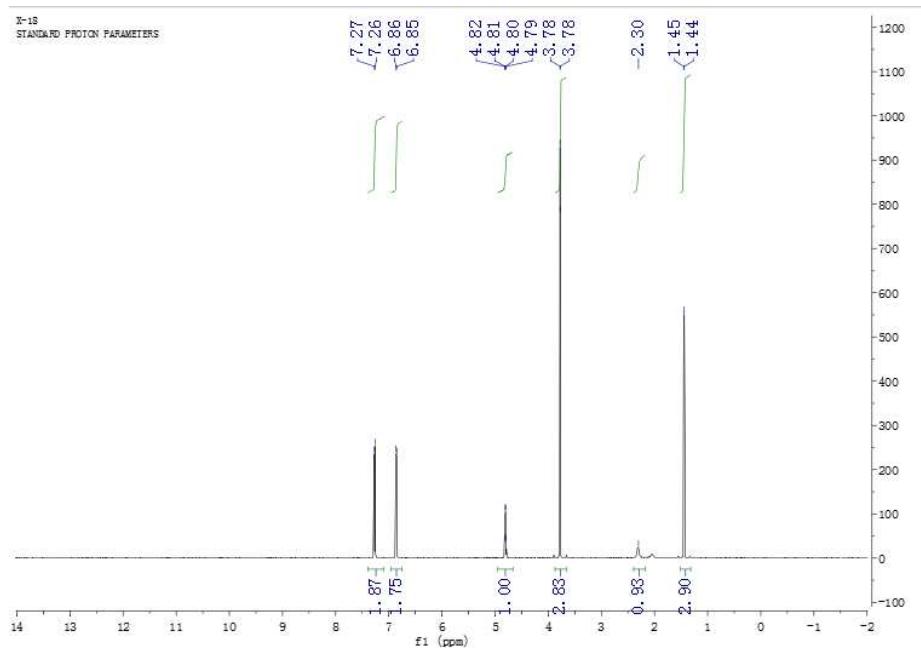
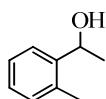
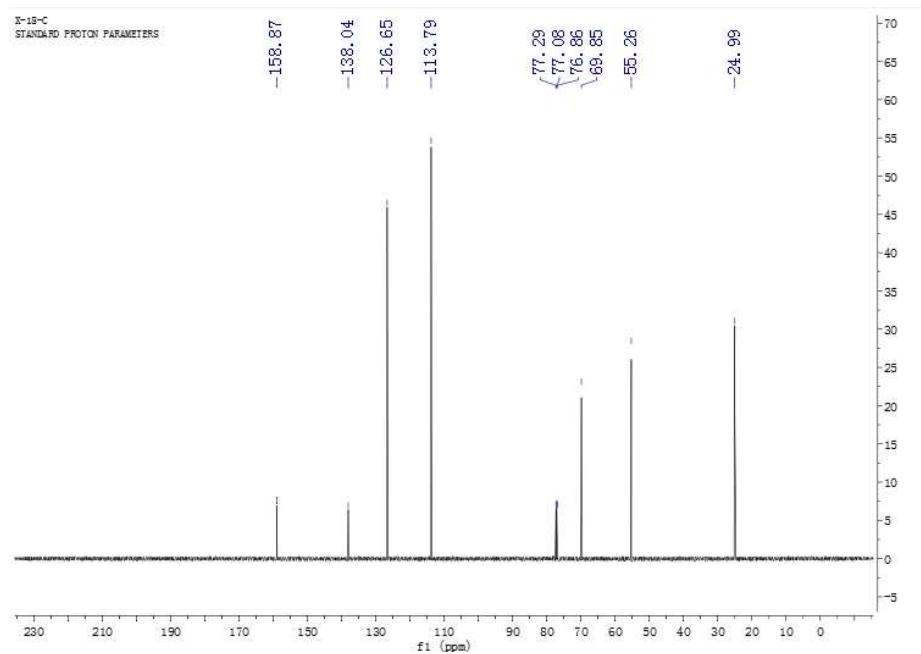
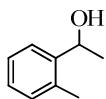


Figure S42 ^{13}C NMR of compound



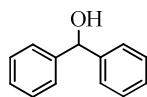


Figure S43 ^1H NMR of compound

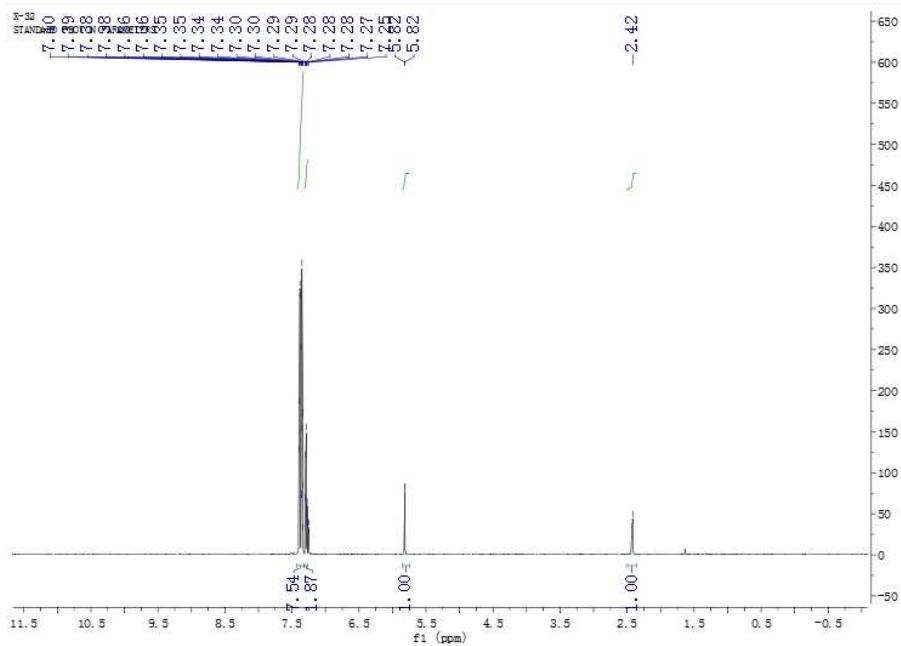


Figure S44 ^{13}C NMR of compound

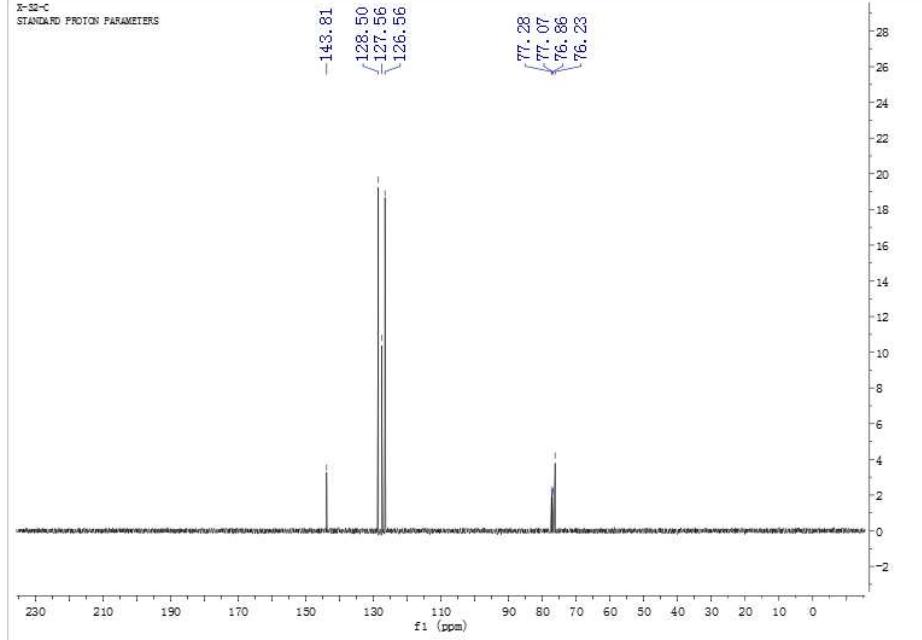


Figure S45 ^1H NMR of compound

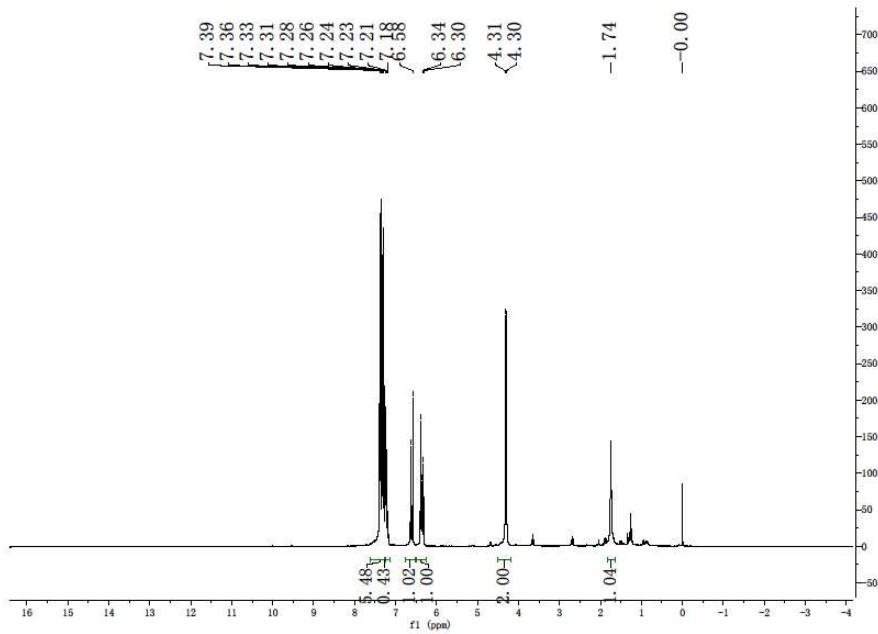


Figure S46 ^{13}C NMR of compound

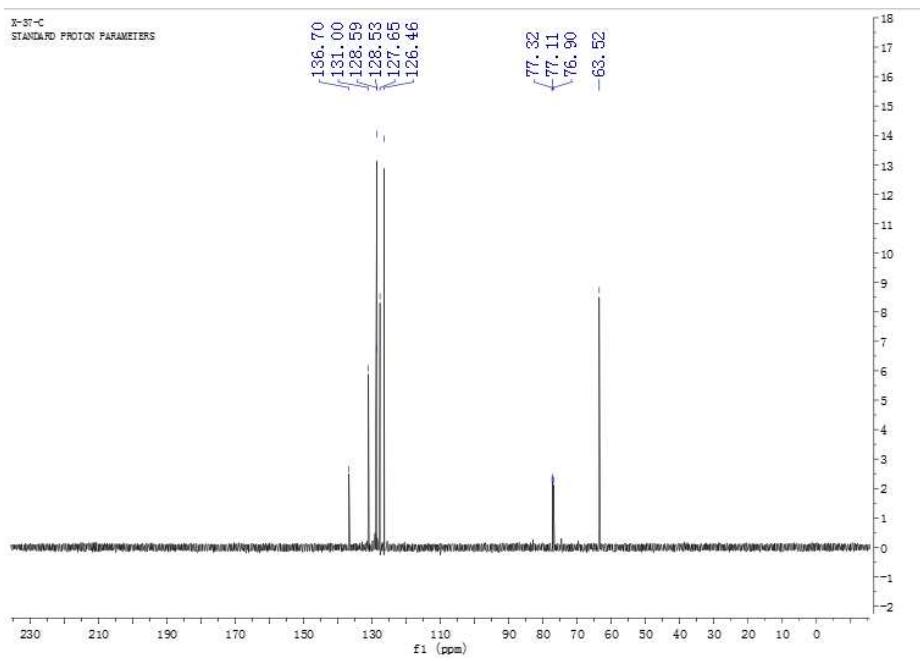


Figure S47 ^1H NMR of compound

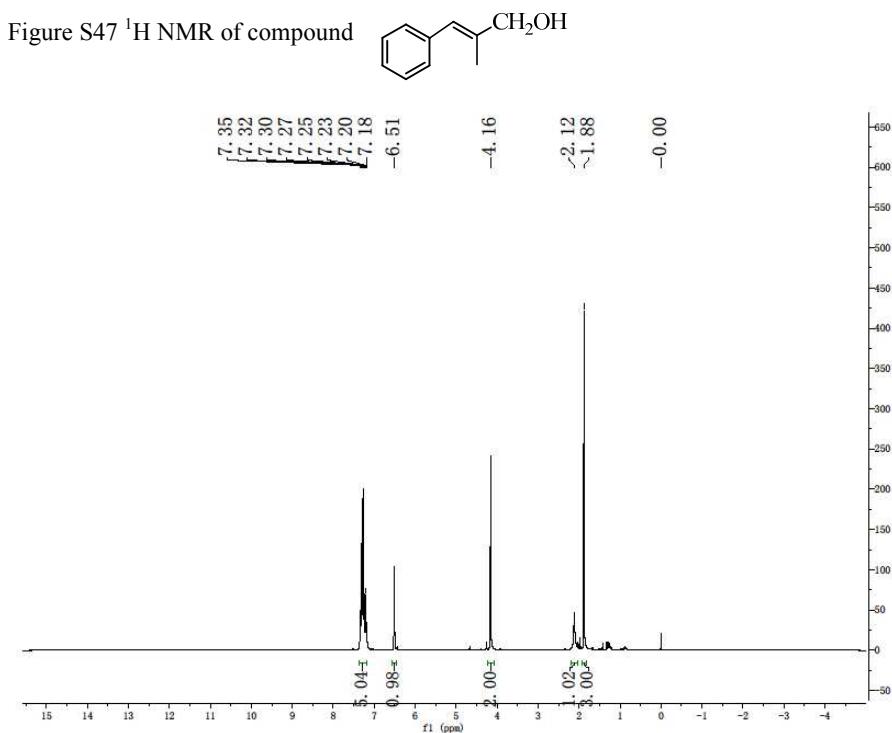


Figure S48 ^{13}C NMR of compound

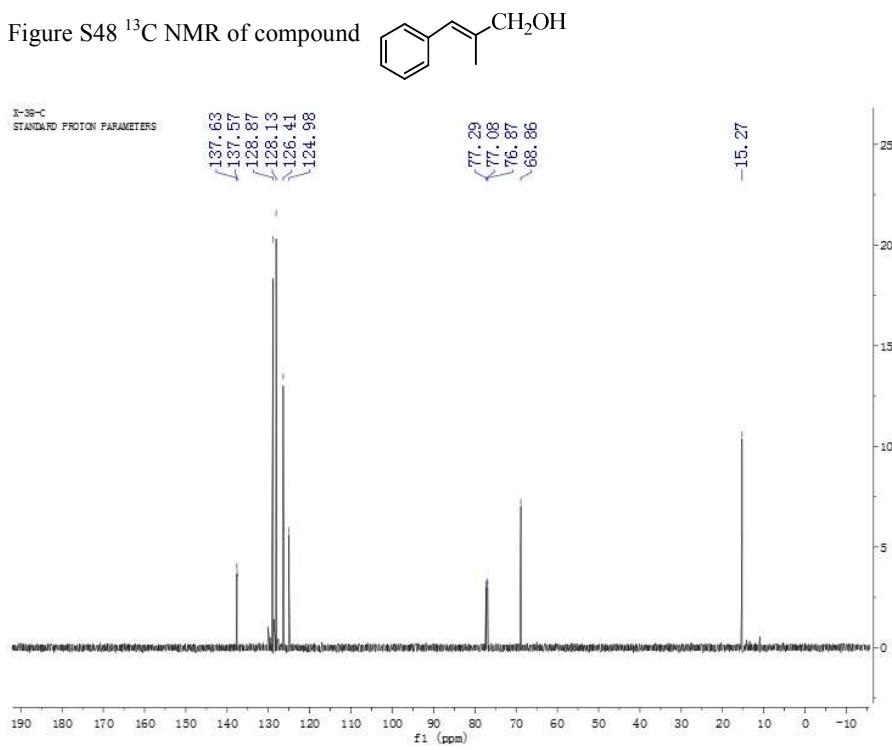


Figure S49 ^1H NMR of compound

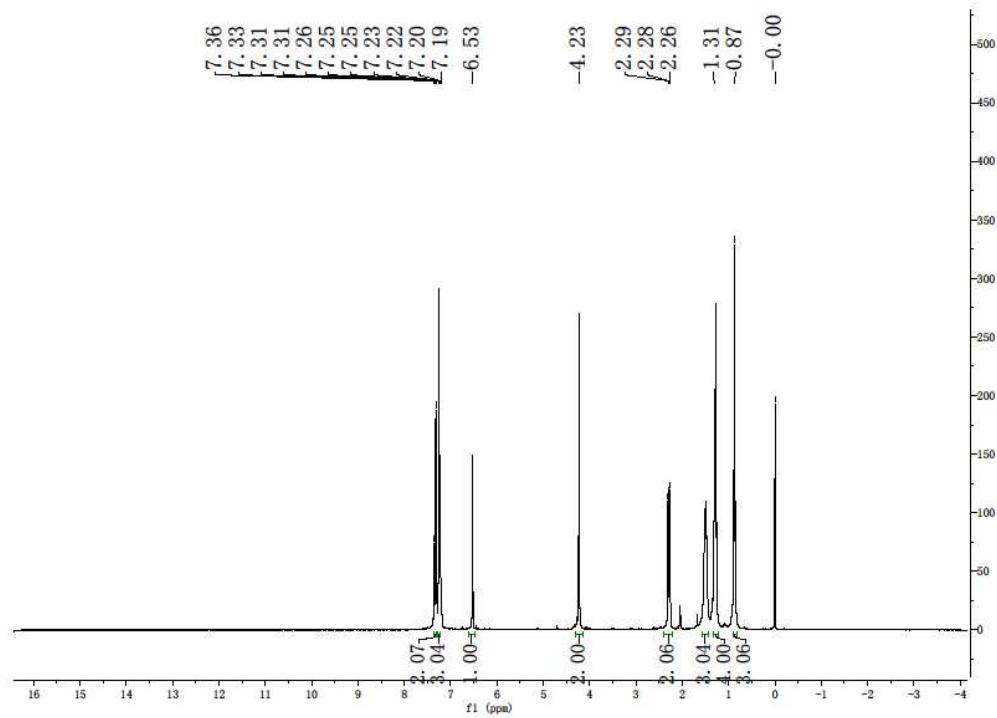


Figure S50 ^{13}C NMR of compound

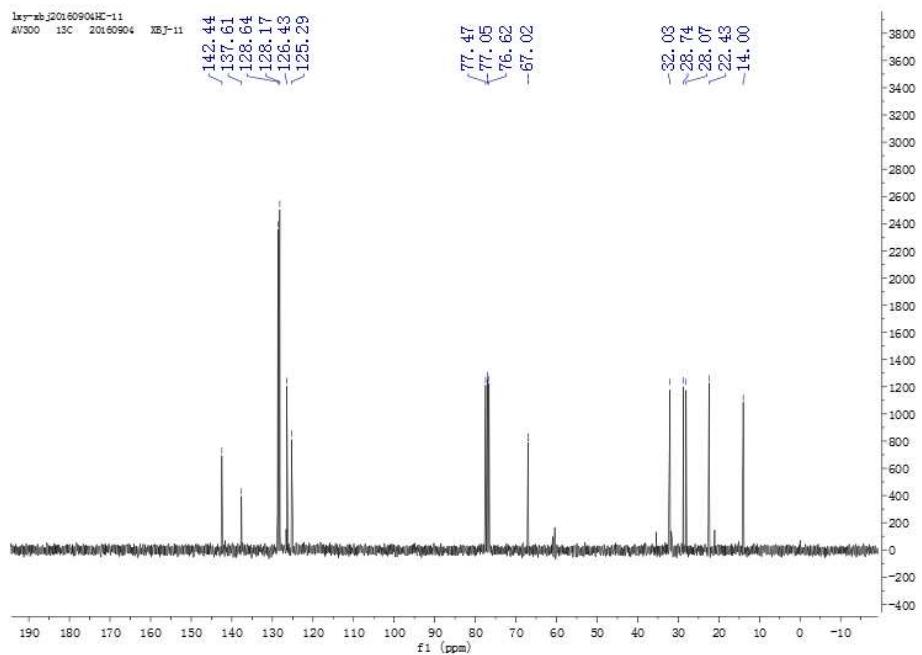


Figure S51 ^1H NMR of compound

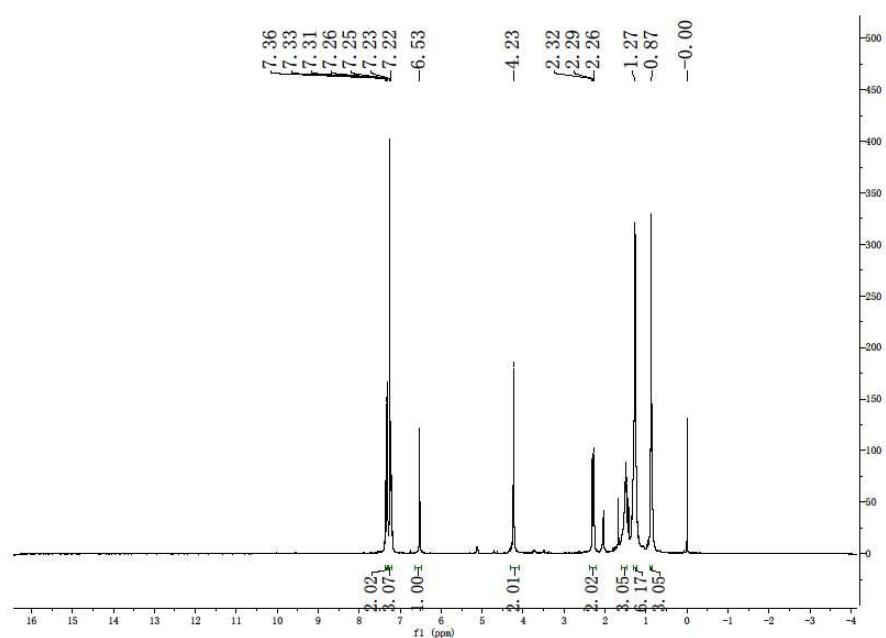


Figure S52 ^{13}C NMR of compound

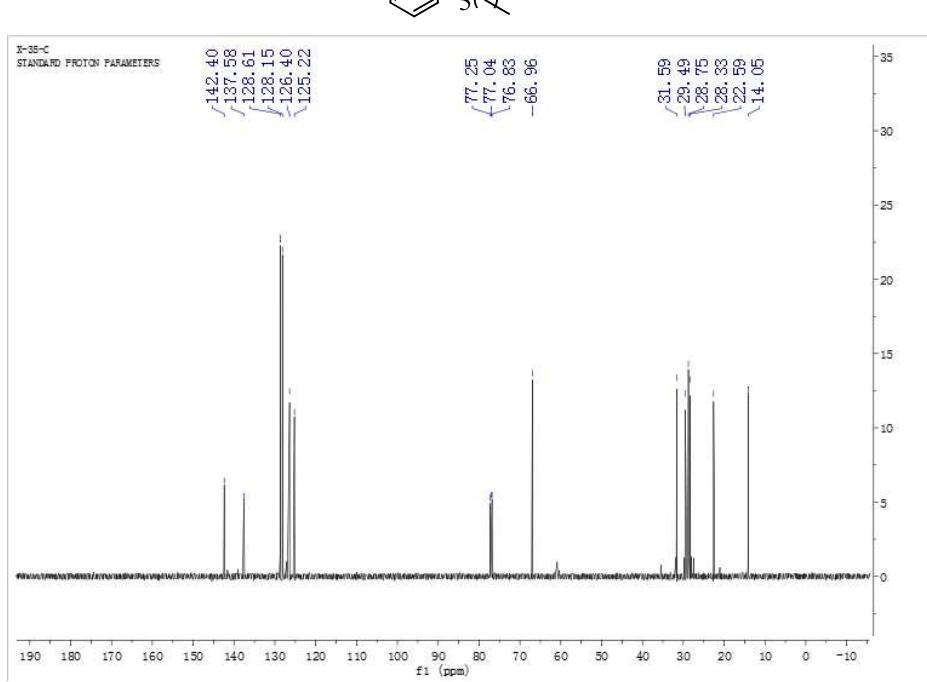


Figure S53 ^1H NMR of compound

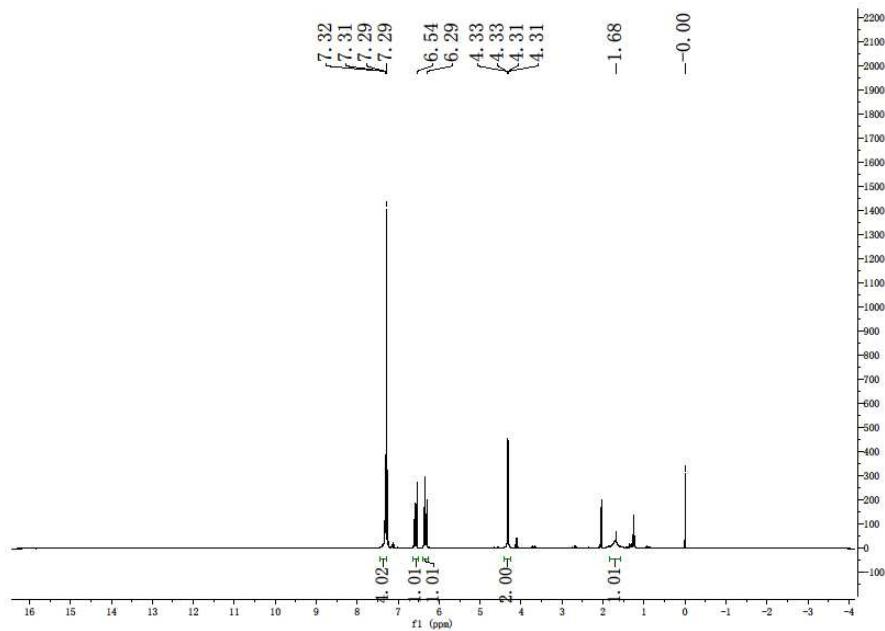
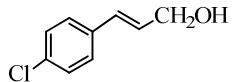


Figure S54 ^{13}C NMR of compound

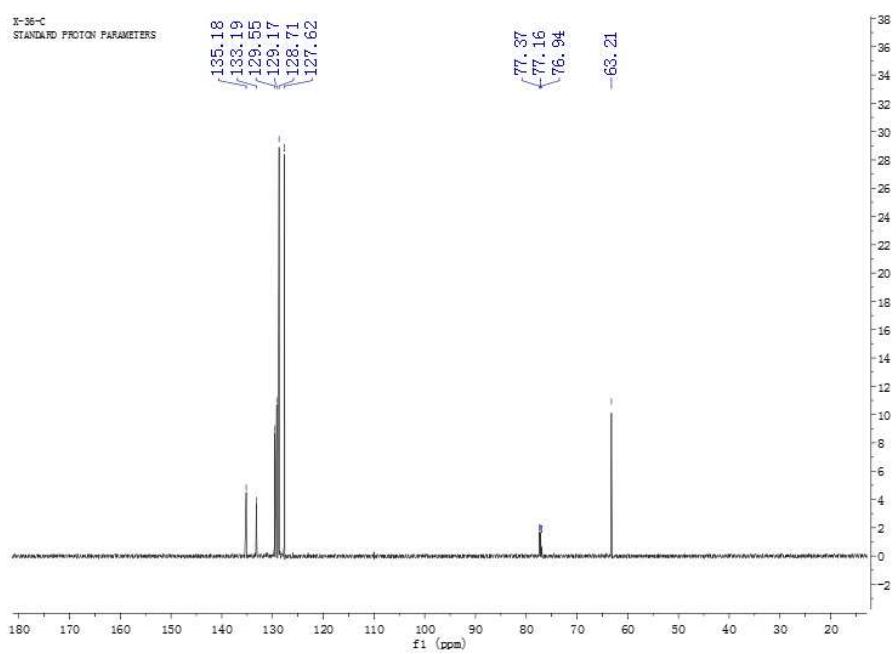
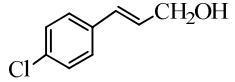


Figure S55 ^1H NMR of compound

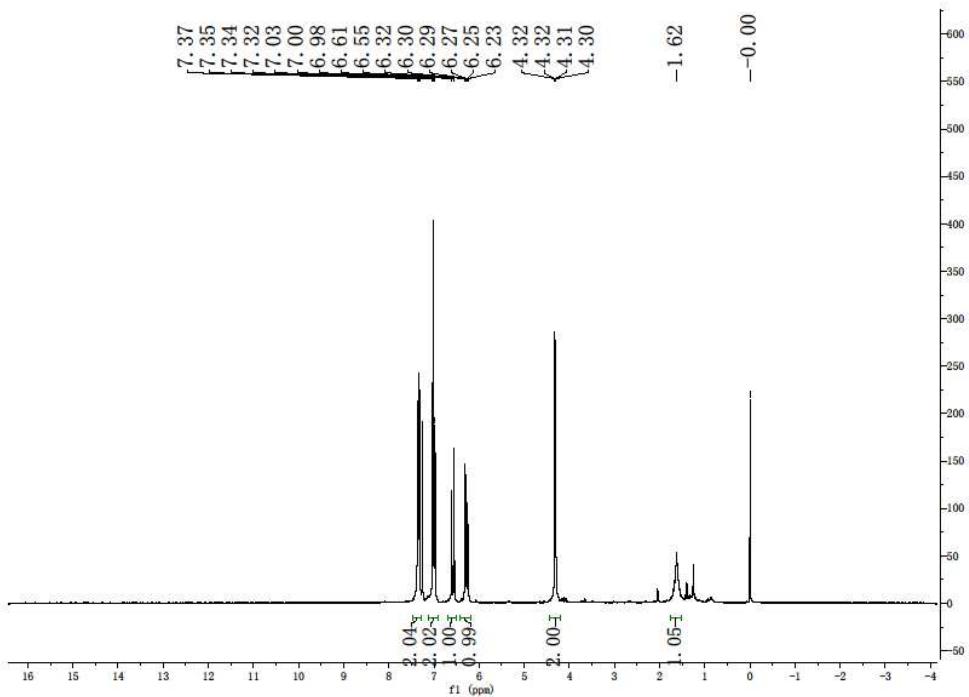
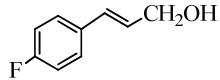


Figure S56 ^{13}C NMR of compound

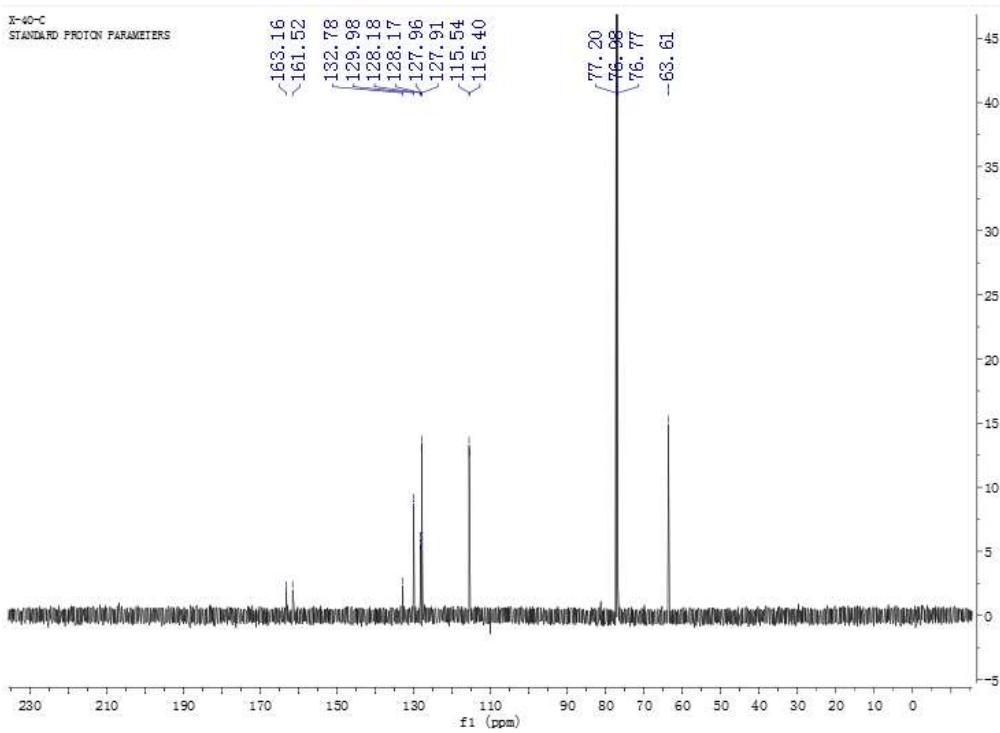
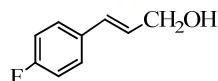


Figure S57 ^1H NMR of compound

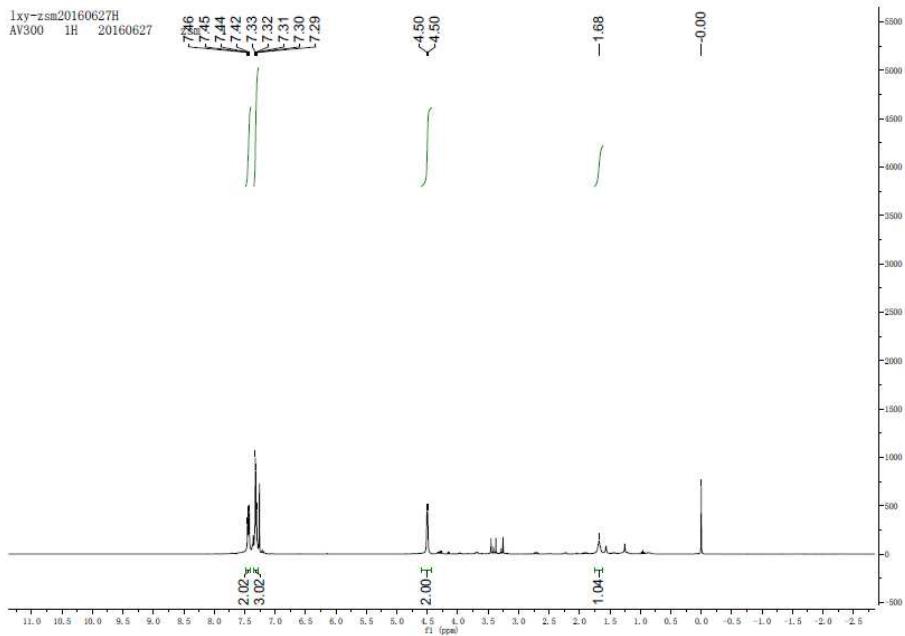
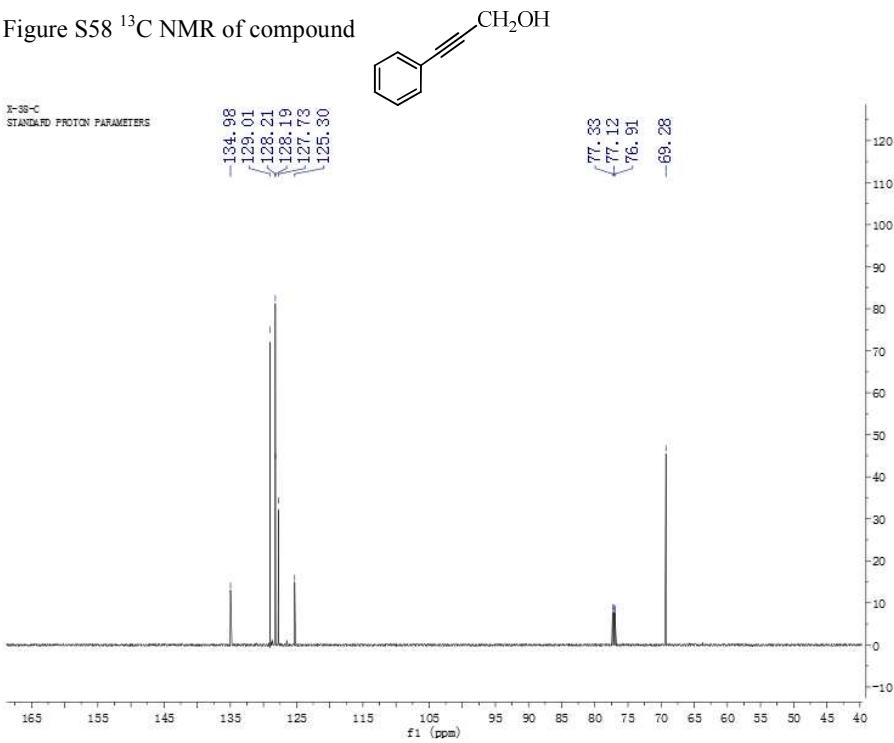


Figure S58 ^{13}C NMR of compound



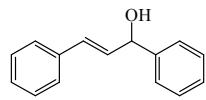


Figure S59 ^1H NMR of compound

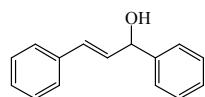
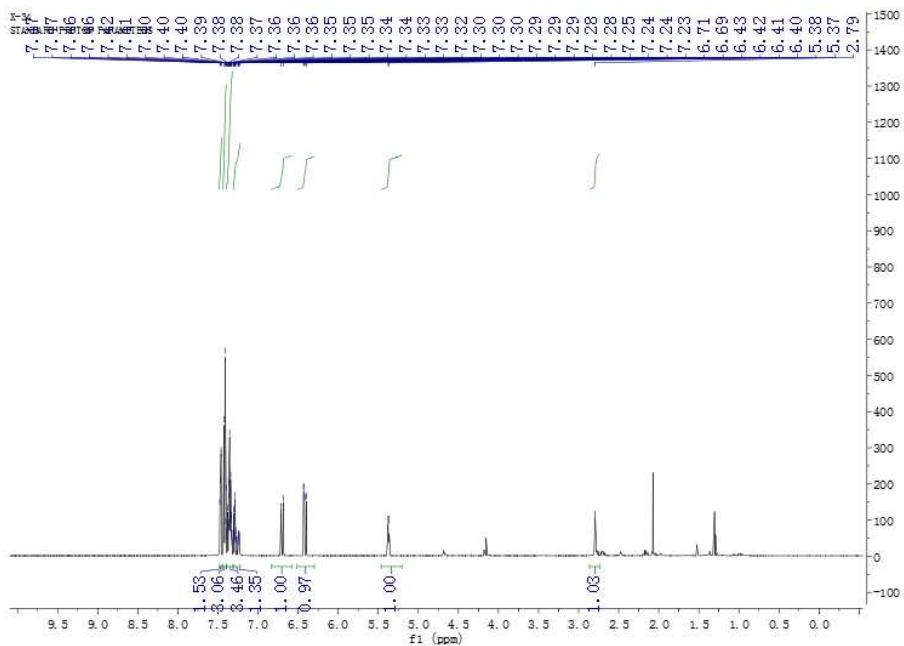


Figure S60 ^{13}C NMR of compound

